

**The research topics
of the Doctoral School of
PHYSICS
at University of Debrecen,
Hungary**

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I. Atomic- and molecular physics program

Supervisor: **Dr. Ágnes Nagy**

PF1/43-93

Density functional theory

Density functional theory is a theory of electronic structure of atoms, molecules, solids and clusters that involves the electronic density as basic unknown, not the electronic wave function. This constitutes an immense simplification, the former being a 3-variable quantity, the latter a 4N-variable quantity, Research will be carried out on various aspects of the density functional theory:

- study of exchange-correlation and kinetic energy functionals
- kinetic energy, Pauli energy, Pauli potential
- calculation of excitation energies
- pseudopotential in the density functional theory
- "thermodynamical formalism" of the density functional theory

Supervisor: **Dr. László Sarkadi**

PF1/410-93

Investigations of forward electron emission in atomic collisions

The subject is related to one of the old problems of the atomic physics. The root of the problem is the long range nature of the coulomb force, which in some cases represents an enormous difficulty for the theoretical interpretation. Such a case is the so-called "cusp" peak appearing in the energy spectrum of the electrons emitted in atomic collisions in the direction of the particle beam.

The properties of the cusp have been extensively studied by the atomic physics group of ATOMKI in the past years. The investigations have raised several questions whose answering can be, among others, the purpose of a doctoral research work, too. The candidate will work on the following two main problems:

1. One of the most significant results of the group was achieved by applying neutral atoms as projectiles. The observations could be explained theoretically assuming that part of the atoms (He) in the neutral beam was in excited metastable state. A recent experiment has proved this assumption. Further experiments using a beam of metastable He atoms of almost 100 % purity are needed to get data which can be directly compared with the theoretical calculations.

2. Another direction of the cusp studies in ATOMKI is the research of the electron correlation, which belongs to the hot topics of the physics of energetic atomic collisions. At present this subject is studied by observation of such processes, where two electrons are activated during the collision. At the same time, the electron correlation can be effectively examined using the method of the electron spectroscopy by means of excitation of atomic resonance states, too. In the vicinity of the cusp resonances of the projectile even with quite small transition energies (about 10 meV) can be identified. In a preliminary experiment the atomic physics group has observed several unknown autoionisation peaks in the spectrum of the cusp of singly charged positive carbon ions. The research task in this field is the systematic study of the properties of the resonances and the possible ways of their excitations

for a series of light and heavier ions (atoms) which can be obtained from the 1.5 MV Van de Graaff accelerator of the Institute.

Supervisor: **Dr. Béla Sulik**

PF1/422-96

Detailed study of the ionization processes by measuring multiple differential electron ejection cross section in ion-atom collisions

This study is predominantly experimental and fundamental. It is planned to achieve a better understanding of ionisation processes in atomic collisions. The main difficulties in describing the inelastic ion-atom collision processes are related to the long-range character of the Coulomb force. For the development of atomic collision theory, it is essential to perform accurate, differential measurements.

When the projectile is an ion carrying electrons, the collision process is rather complicated. The spectrum contains electrons ejected from both the target and projectile centres. To separate the different contributions one needs to measure the electrons in coincidence with the charge state of the scattered projectile ion. The interpretation of the double differential (according to the angle and energy of the ejected electron) electron spectra taken in coincidence with the projectile charge state needs the full arsenal of atomic collision theories. A high level of understanding is essential for both fundamental physics and applications.

The object of the planned study is the experimental determination of the full angular and energy distribution of electrons ejected from 50-150 keV/u C^+ , N^+ + He, Ne, Ar collisions in coincidence with the charge state of the scattered projectile ions. We intend to perform a rather complete interpretation. In the first phase of the work emphasis is given on the projectile electron loss process at backward angles. From a theoretical point of view this is the most interesting region.

Neglecting some preliminary measurements, the study starts in 1996. It is a unique possibility for the PhD student to take part in a fundamental research work from the beginning. The work is mostly experimental. One needs to learn high level experimental methods and apparatus. Part of the experiments are to be performed in international collaborations.

Supervisor: **Dr. Sándor Biri**

PF1/427-03

Investigation of highly charged heavy ion plasmas

During past years an Electron Cyclotron Resonance (ECR) Ion Source was built and put into operation in the ATOMKI. This way the first particle accelerator to generate highly charged heavy ion beams in Hungary and in Central-Europe, was established. The ion source is able to produce strongly ionised plasmas and any charged, low energy beam from most elements of the periodical table (<http://www.atomki.hu/ECR>).

Experimental plasma and atomic physics research can be performed with the ion source and, partly, on the ion source itself. The main purpose of these research is to study this unusual material which is hardly produced by other methods in laboratories. Direct and indirect diagnostic methods can be used (Langmuir-probes, visible light and X-ray detectors)

and many physical parameters (e.g. ion charge state distribution, plasma potential, electron density and temperature, atomic levels) can be investigated this way. The necessary instruments (detectors, spectrometers, computers) are available in the ATOMKI, in the DE-KFI or at our partners abroad. The second research topic is production of fullerene plasmas and beams by new methods, production and investigation of endohedral fullerenes (they contain an alien atom in their centre, e.g. N@C60). These topics require the supervised operation of the ECR facility.

The ECR group developed a PC-code to simulate magnetic traps and partly the elementary processes in such traps (charged particle movement, electron cyclotron resonance etc.). The main purpose of this research by systematically running this code is to simulate different ion traps (not only ECR) and the results of planned and executed experiments.

Supervisor: **Dr. Károly Tókési**

PF1/428-03

Interaction of charged particles with atoms and surfaces

The recent availability of sources for slow highly charged ions (HCI), namely electron cyclotron resonance (ECR) and electron beam ion sources (EBIS) has led to a flurry of research activities, both experimental and theoretical, in the field of HCI-solid interactions. On the most fundamental level, its importance is derived from the complex many-body response of surface electrons to the strong Coulomb perturbation characterized by a large Sommerfeld parameter $\eta = Q/v \gg 1$ (Q : charge of the incident HCI, v : velocity). Moreover, the study of multiply-charged ion – solid interactions is also of considerable technological importance for the understanding of material damage, surface modification, and plasma-wall interactions. Interactions of multiply charged ions with solids explore a parameter regime significantly different from singly or doubly charged ions. Most importantly, the neutralization is a true multi-electron capture (and loss) process involving up to the order of ≈ 100 electrons and posing a considerable challenge to theory. Furthermore, resonant transfer processes involve highly excited levels in the ion far away from the ground state. They are expected to set in at large distances from the surface, R , when the atomic wavefunction begins to *touch* the surface. This simple picture suggests the probing ion-surface interactions at large distances involving Rydberg states (large quantum numbers, $n \gg 1$ which lends itself to an approximate (semi)classical description of the electronic degrees of freedom.

The theoretical description of this new class of processes is far from being well understood. Earlier descriptions rely on classical dynamics which have proven to be quite successful in comparison with experimental data. However, since very detailed measurements have recently become available, critical and precise tests are only now being possible. Performing detailed tests of classical theory and developing a quantum many-body theory for highly charged ion - solid interactions are the main goals of this project.

Supervisor: **Dr. Béla Sulik**

PF1/429-06

Relativistic atomic physics at storage rings

The topic is connected to the planned development (Facility for Antiprotonic and Ionic Research, FAIR, <http://www.gsi.de/fair>) of one of the most important centers of high energy atomic and nuclear physics, the “Gesellschaft für Schwerionenforschung” (GSI), Darmstadt,

Germany. The development of the new accelerator – storage ring complex and the formation of one of the user’s “group” (Stored Particle Atomic Physics Research Collaboration, SPARC, <http://www.gsi.de/fair/experiments/sparc/>) undergoes in a wide international collaboration. Within the SPARC collaboration, in the forthcoming 4-5 years, the main activity is the development of the experimental apparatus, including different spectrometers. In the future, the developers and their home institutions gradually become the (high priority) users of the apparatus, conducting atomic physics research at FAIR/GSI.

Our Institute, ATOMKI, together with the University of Debrecen, is interested to play some role in the development and construction of two huge magnetic electron spectrometers (http://www.gsi.de/onTEAM/grafik/1068560945/TR_ELOI.pdf) and a so called „reaction microscope”, a specific combination of ion and electron spectrometers, which is able to determine the momentum vectors of all particles emerging from an atomic collision (<http://www.gsi.de/fair/experiments/sparc/coltrims.html>). We would like to delegate one (or two) Ph.D. students to Darmstadt whom should participate in this work. The Ph.D. student(s) would make the work under the joint supervision of the University of Debrecen, GSI and the University of Giessen. During the Ph.D. period, the Ph.D. student(s) should

- perform calculations for planning the high resolution, high accuracy magnetic electron spectrometer giants, working in the far relativistic electron velocity regime. He or she will learn and work with the highest rank programs for calculating charged particle trajectories in combined electric and magnetic fields (e.g., OPERA, TOSCA).
- perform calculations for planning the reaction microscope (SIMION, OPERA, TOSCA)
- participate in presently running atomic physics experiments at GSI (e.g, ionization of one or two electron ions, dielectronic recombination, radiative capture, test measurements for QED, etc.).

The proposer supervisor (sulik@atomki.hu) can be asked for detailed information.

Supervisor: **Dr. Ágnes Vibók, Dr. Gábor Halász**

PF1/431-08

Photo-induced nonadiabatic quantum molecular dynamics

Molecules are composed of fast moving light electrons and slow moving heavy nuclei. One very commonly used approximation in the theoretical description of these systems is the so called Born-Oppenheimer (BO) or adiabatic approximation introduced by Born and Oppenheimer in 1927. They separated the motion of fast electrons and slow nuclei in a quantum mechanical framework. This approximation is frequently accurate enough to allow the detailed understanding and prediction of molecular properties and processes. It turns out, however, that the approximation is valid only if the nuclear configuration is such that the electronic energies are well separated. Nuclear configurations where two electronic energies are equal (i.e. the corresponding states are degenerate) are points (CI, Conical intersections) where the approximation breaks down. In this case the so-called non-adiabatic transition goes on between the adiabatic electronic states by allowing for the motion of nuclei to move on coupled multiple adiabatic electronic states.

There is a large class of biologically, chemically and physically interesting processes (for instance most of photochemical reactions) in nature, where the system exhibits degeneracy and hence the non-adiabatic description is justified. Conical intersections exist already between low lying electronic states of small molecules. The number of them will increase if one increases the number of atoms or the number of electronic states studied in the molecule. Therefore one has to practically take into account large number of CIs in

polyatomic molecules which provide pathways for fast interstate crossing. The short-time dynamics always takes place through a conical intersection.

Supervisor: **Dr. Béla Sulik**

PF1/434-08

Atomic and molecular collisions relevant for radiation damages in bio-molecules and some ion technology processes

We study ion-atom and ion-molecule collisions which play significant role in radiation damages of small and large molecules in biological tissues. This is important for cancer therapy methods by energetic ion bombardment. Moreover, some of these processes gain importance in understanding ion-solid interactions better. We study the fragmentation of small molecules by ion impact in details, and the specific mechanisms of fast electron production during the slowing down of ions in matter. These phenomena are studied by the small and medium energy accelerators of ATOMKI, Debrecen. Part of the work is performed in international collaborations. The PhD student is expected to participate in the experiments, to conduct experiments alone in a later stage of the work, and to participate in the theoretical interpretation.

The supervisor (sulik@atomki.hu) can be asked for detailed information.

Supervisor: **Dr. Béla Sulik**

PF1/435-08

The interaction of insulator nanocapillaries with ions: Ion-beam guiding and focusing

The topic is the study of a recently (2002) discovered phenomenon, and promote its applications. Nanocapillaries of 50-200 nm in diameter, formed in insulator foils are capable to deflect highly charged, keV energy ions by 5-25 degrees in direction. The phenomenon is based of the **self organizing** charge-up of the inner capillary walls. We study these processes at the beam line of the electron cyclotron resonance (ECR) ion source of ATOMKI, Debrecen. Part of the work is performed in international collaborations. Our future aim is to create small ion-focusing elements for keV energy ions from curved insulator foils. The PhD student is expected to participate in the experiments, to conduct experiments alone in a later stage of the work, and to participate in the model calculations for the theoretical interpretation.

The supervisor (sulik@atomki.hu) can be asked for detailed information.

Supervisor: **Dr. Gábor Halász**

PF1/436-08

The role of degeneracy in molecular systems

Molecules are composed of fast moving light electrons and slow moving heavy nuclei. One very commonly used approximation in the theoretical description of these systems is the so called Born-Oppenheimer (BO) or adiabatic approximation introduced by Born and Oppenheimer in 1927. They separated the motion of fast electrons and slow nuclei in a quantum mechanical framework. This approximation is frequently accurate enough to allow the detailed understanding and prediction of molecular properties and processes. It turns out,

however, that the approximation is valid only if the nuclear configuration is such that the electronic energies are well separated. Nuclear configurations where two electronic energies are equal (i.e. the corresponding states are degenerate) are points (CI, Conical intersections) where the approximation breaks down. In this case the so-called non-adiabatic transition goes on between the adiabatic electronic states by allowing for the motion of nuclei to move on coupled multiple adiabatic electronic states.

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Supervisor: **Dr. Ágnes Vibók**

PF1/437-11

Laser-induced nonadiabatic processes in molecular systems

Conical intersections (CIs) between electronic potential energy surfaces play a key mechanistic role in nonadiabatic molecular processes. In this case the nuclear and electronic motion can couple and the energy exchange between the electrons and nuclei becomes significant. CIs appear between different electronic states starting from triatomic systems to truly large polyatomic molecules. Conical intersections can also be formed by laser waves. In this case the laser light induces CIs which couple the electronic states and the internal rotational and vibrational motions. The light-induced CIs constitute a novel and physically interesting new laser-matter phenomenon. The presence of these light-induced CIs in molecules may completely change their original, i.e., field free, physical properties. In other words, using either standing or running laser waves or laser pulses, it is possible to generate significant nonadiabatic effects in molecular systems. Application of external fields thus opens up a new direction in the area of quantum dynamics and also of control of molecular processes. The light-induced nonadiabatic effects have the ability to couple in a controllable way different electronic states of molecules. Depending on the field intensity, the nonadiabatic coupling can be extremely large in the vicinity of the CIs.

The aim of this PhD work is to investigate the effect of the light-induced CI for the different physical properties (photodissociation probabilities, alignments etc...) of diatomics and triatomics.

The subject is theoretical, but we plan to collaborate with experimental groups, in order to apply the obtained concept and results.

Supervisor: **Dr. Ágnes Nagy**

PF1/439-13

Quantum phase transitions, classical and quantum chaos

The quantum phase transitions take place at zero temperature. Contrary to the classical phase transitions, quantum phase transitions are driven by quantum fluctuations. Quantum phase transitions are often studied by models (e. g. Dicke, vibron) with Hamiltonian

$H = h + \lambda V$, where h is integrable. At a special value of the control parameter λ , an abrupt change is taking place in the system.

In the Dicke model it was demonstrated that at the transition point the system changes from being quasi-integrable to quantum chaotic. The linearity of quantum mechanics precludes chaos in the classical sense. Quantum chaos is quantum mechanical description of classically chaotic systems. Quantum phase transitions are often precursors of the emergence of quantum chaos. Research aims at quantum phase transitions, classical and quantum chaos and their relationship.

Supervisor: **Dr. Ágnes Vibók**

PF1/441-14

Photo-induced electron and nuclear dynamics in molecules on an attosecond to few femtosecond time scale

Considerable advances in the pump-probe techniques utilizing femtosecond and sub-femtosecond pulses made possible to control complex molecular dynamical processes. The appearance of attosecond extreme-ultraviolet pulse has newly brightened up the hope for controlling electronic motions as well. Attosecond pulses have opened the door to study processes, among others such as ultrafast charge migration after sudden ionization, ultrafast exciton migration after coherent superposition of electronic states in molecular system.

The main goal is to study the coupled electronic and nuclear dynamics in molecular systems containing few atoms. Within this project the applicant has to develop a theoretical approach to interpret the experimental data. Among others she/he has to calculate the time-dependent molecular dipoles, the time resolved photoelectron spectra (TRFES) and the molecular frame photoelectron angular distributions (MFPADs).

Supervisor: **Dr. László Gulyás**

PF1/442-15

Many-electron processes in simple atomic and molecular collisions

The recent development of the reaction microscope has opened a new chapter in the field of atomic and molecular collisions. Kinematically complete measurements have been available for detailed investigations of the various reaction mechanisms which are real challenges for the theoretical descriptions. In many collision processes the contribution of many-electron transitions are not negligible. The independent electron model provides a simple tool for describing multi-electron transitions, however, the accurate knowledge of single electron

transitions (excitation, ionization, electron capture by the projectile ion) is very important to get a realistic estimation on the possible role electron correlation in the process studied.

In this project multi-electron processes will theoretically be investigated in simple atomic (Z^{q+} - He, Li, Ne,...) and molecular (Z^{q+} - H₂, H₂O, CH₄,...) collisions at medium and high impact energies where perturbative treatments are suitable. The single-electron transitions will be accounted for within the framework of distorted wave formalism. The role of static (correlation in the “unperturbed” region) and dynamic (in the course of collision) correlations and, in the case of molecules, fragmentation routes will approximately be included in the formalism.

Supervisor: **Dr. Zsolt Mezei**

PF1/443-19

Elementary molecular processes in the cold ionized media

The cold ionized media, i.e. the interstellar molecular clouds, the supernovae, the planetary atmospheres, cold laboratory and fusion plasmas etc., containing molecular species are the seat of an extremely rich chemical physics, mainly due to the presence of electrons, cosmic rays, photons and neutral and ionized species in excited states. The successful modelling of these non-equilibrium environments is critically based on the precise knowledge of state-to-state cross sections and/or rate coefficients of the dominant radiative or collisional elementary processes. In particular, a special interest goes to the branching ratios of these processes, since it provides the most detailed description of the level population and of the chemical composition of these environments [1].

The presence of several fragmentation continua - electron/molecular-ion (ionization), neutral/neutral (dissociation), cation/anion (ion-pair) - and the non-adiabatic couplings between the motion of electrons and of the nuclei make these collisions extremely challenging to treat.

The present research project deals with the astrophysically relevant molecular ions - recently discovered in the interstellar medium (HCl⁺, SH⁺ [2], N₂H⁺), or species planned as fuel for the electric propulsion of satellites and space crafts (I₂⁺ [3]). It includes electron structure and spectroscopic calculations of neutral and charged molecular species (standard quantum chemistry and R-matrix based methods), and the nuclear dynamics of the reactive collision processes (multichannel quantum defect theory, MQDT [4]), which in turn relies on precise molecular data – the adiabatic and/or diabatic potential energy curves of bound (ground, excited and super excited) and dissociative states of the molecule and of the molecular ion, as well as coupling between the ionisation and dissociation continuum of the molecule.

[1] E. Roueff, EPJ Web of Conferences 84, 06004 (2015).

[2] D. O. Kashinski, et al, I. F. Schneider and J. Zs. Mezei, J. Chem. Phys. 146, 204109 (2017).

[3] P. Grondein et al, Phys. Plasmas 23, 033514 (2016). [4] Ch. Jungen, in Handbook of High Resolution Spectroscopy, Wiley, Chichester, New York (2010).

Quantum correlations in molecular systems

Quantum informatics lies at the crossroads of quantum information theory and quantum physics, which harnesses puzzling quantum phenomena offered by encoding information into quantum particles. Novel applications become available such as quantum computers, quantum simulators, and secure quantum communication. Quantum informatics may hold the key for a technological revolution. At the heart of these applications is nonclassical correlations arising between entangled quantum particles. In recent years due to technological advances higher dimensional entangled states can be routinely created and such states potentially offer new perspectives to applications, such as quantum cryptography.

In the present programme, we aim at quantifying higher dimensional entanglement. The PhD student will take part in the theoretical study of quantum correlations originating from higher dimensional two-fermionic systems. Special focus will be given to the following topics:

- (i) Devising and implementing an efficient numerical tool based on semidefinite programming relaxations to bound the Slater number of indistinguishable particles;
- (ii) Producing so-called Slater witnesses with the application of our numerical tool above;
- (iii) Application of the devised methods and tools to specific two-electronic molecular systems.

Certification of quantum information applications

Recent technological advances on the control of quantum systems is paving the way for a quantum revolution that would guarantee communication security, enable quantum simulation of chemical processes and yield unprecedented computing power. However, it also sets great challenges regarding the certification task that these quantum devices and protocols operate according to specification. Indeed, given a quantum device, how could the user of this device make sure that it performs a certain computational problem correctly? This quantum certification task stands out as a key aspect in the EU Quantum Technologies Program as well.

In the present research programme, the Ph.D. student will address quantum certification of various quantum information applications, which can be implemented with available technologies. In particular, the Ph.D. student will develop the concepts and devise efficient methods to certify (1) many-body quantum systems, (2) high-dimensionally entangled systems, and (3) quantum networks. In case (1), the objective is to construct protocols which detect nonlocal correlations in many-body systems and benchmark quantum simulators. In case (2), the objective is to certify genuine high-dimensional quantum properties such as entanglement with various degrees of trust in the quantum devices. In case (3), the objective is to exploit the genuine quantum effects which arise when quantum particles are distributed in a network topology. Collaboration with experimental groups regarding the implementation of the above tasks is also foreseen.

Modelling of atomic processes in fusion plasma

The recently used energy production methods will not be able to satisfy the energy needs of humanity in the long run. In the absence of a rapid increase in energy storage efficiency, it is becoming increasingly urgent to develop an environmentally friendly, regulate solution of the new energy source. One of the best solutions in future would be the implementation of fusion power plants.

Therefore the main purpose of the PhD study is to study the interaction of fusion plasma with matter, which involves the interaction of ions and wall and the interaction between plasma and various ions. The focus of our investigations is the study of the energy and angular distribution of the ions in ion-atom and ion-surface collisions and the fusion chamber damage during ion irradiation. Specifically, we look for the answers to the following specific questions:

a) In the case of Be, Fe and W atoms forming the wall of the fusion chamber (and also for H, Ne, and Ar and other atoms present in the fusion plasma), detailed calculations are planned for each atomic shell to determine the ionization and capture cross sections for H, D, T, H^+ , D^+ , T^+ projectiles. To make the calculations, we will use the different versions of the classic Monte Carlo and quantum mechanical methods.

(b) Along the plan a) we determine the energy and angular differential cross sections for H, D, T, Be, Fe, and W targets and for He, He^+ and He^{2+} projectiles.

Requirements: Basic knowledge of atomic physics. Quantum and classical physics.

Knowledge of programming language (Fortran, C, C++, etc).

Good skill of manuscript writing in English.

Ultracold molecular gases

The proposed research topic is related to the rapidly growing research field of ultracold

(< 1 μ K) quantum gases. Such systems are expected to play a major role in future quantum technologies, which is one of the flagship projects supported by Horizon 2020. This direction of the research illustrates one of the current trends of modern atomic, molecular, and optical physics joining condensed matter physics with ultracold quantum degenerate atomic and molecular systems. The developments and achieved results in this domain resulted in a series of Nobel Prizes: laser cooling of atoms (2007 Prize) which paved the way towards the first observation of Bose-Einstein condensation in dilute gases (2001 Prize), the 2003 Prize for contribution to superconductivity and superfluidity theory, followed by the 2005 Prize for optical frequency combs, and the 2007 Prize in Chemistry for coherent control.

Ultracold molecules due to their richer internal structure compared to atoms offer more possibility for external manipulations and control of quantum systems. Such systems are important for quantum information devices, entanglement tests, quantum simulators, quantum degeneracy, precision measurements for testing fundamental theories, high-resolution molecular spectroscopy and elementary chemical reactions.

Unlike atomic gases the density of ultracold ground state molecular gases has not yet been attained experimentally to reach quantum degeneracy. The present project is strongly related to experimental realization of ultracold molecular quantum gases when the molecule is formed from two alkali metal atoms (eg. KCs) or from an alkali metal and an alkaline earth metal atom (eg. RbSr). In the present project the proposed molecular structure calculations [1, 2, 4] have importance in the formation of ultracold molecules and their ground state transfer, while semiclassical [3] and quantum calculations regarding ultracold atomic or molecular collisions aim the reduction of inelastic collisions to reach higher molecular densities.

[1] A. Orbán, R. Vexiau, O. Krieglsteiner, H.C. Naegerl, O. Dulieu, A. Crubellier, N. Bouloufa-Maafa, Model for the hyperfine structure of electronically excited KCs molecules, *Phys. Rev. A* 92, 032510 (2015)

[2] R. Vexiau, D. Borsalino, A. Orbán, M. Lepers, M. Aymar, O. Dulieu and N. Bouloufa-Maafa, Dynamic dipole polarizabilities of heteronuclear alkali dimers: optical response, trapping and control of ultracold molecules, *Int. Rev. in Phys. Chem.* 36, 709, (2017)

[3] A. Orbán, O. Dulieu, N. Bouloufa-Maafa, Optical fields to control ultracold atomic/molecular collisions, *Journal of Physics Conference Series* 875, 9 (2017)

[4] A. Orbán, T. Xie, R. Vexiau, O. Dulieu, N. Bouloufa-Maafa, Hyperfine structure of electronically-excited states of the $^{39}\text{K}^{133}\text{Cs}$ molecule, *Journal of physics B: Atomic Molecular and Optical Physics* 52, 135101 (2019)

Supervisor: **Dr. Zoltán Juhász**

PF1/448-19

Experiments on fragmentation of molecules of astrophysical relevance

The molecules in the atmospheres of comets, moons and planets are subject of the damage caused by solar wind and cosmic radiation. Studying such processes at laboratory circumstances is one of objective in the research continued at Atomki. We measure the energy and angular distribution of molecular fragments stemming from collision of ions present in the solar wind and radiation belts with molecules by electrostatic spectrometers and time-of-flight techniques. The applicant has to take part in the experimental work, develop the instruments and interpret and utilize the data in applications.

Supervisor: **Dr. Zoltán Juhász**

PF1/449-19

Spectroscopic investigation of astrophysical ices

An infrared spectrometer with a device producing thin ice layers will be installed at Atomki in a British – Hungarian collaboration. We will study the chemical changes induced by ion impact in ices similar to those present in the interplanetary medium. The accelerators of Atomki allow us to study the chemical effects of solar wind ions and cosmic rays in ices with ground based instruments in a wide energy range. In such processes, complicated organic molecules, which are basic for life, can be created. This will be investigated by space missions, too, in the near future. In order to interpret the data of satellites, ground based experiments are necessary. The applicant is expected to learn the experimental techniques for spectroscopic investigation of ices, perform experiments in collaboration, and be involved in the analysis of the data.

Supervisor: **Dr. András Csehi**

PF1/450-20

Quantum control of molecular processes with classical and quantum light

In the Born-Oppenheimer (BO) picture - which relies on the separation of the movement of fast electrons and slow nuclei - the nuclei move in the effective potential of the electron cloud. These so-called potential energy surfaces are inherent properties of molecules, which dictate the movement of the nuclei. In the presence of periodic external electromagnetic fields, the potential energy surfaces are modified through the dynamical Stark-effect allowing for the control of intramolecular movement by activating or inhibiting certain reaction pathways. By shaping femtosecond laser pulses in the time or frequency domain (e.g. phase modulation, chirping) the nuclear wave packet can be guided via distortion of the potential energy surfaces. On the other hand, the quantum field description of the photon mode allows one to manipulate the light-matter interaction directly in phase space.

In the framework of the proposed PhD work, we plan to carry out highly accurate molecular quantum dynamical simulations of small molecules in the presence of classical and quantum lights. The major goal is to develop an efficient procedure for optimizing electric field forms that induce the molecular motion along predefined quantum pathways. We intend to devote a special care for electronic state degeneracies where the electrons and nuclei are strongly coupled and the BO approximation breaks down. Applying quantum states of light (Fock, coherent, squeezed, and squeezed coherent) we plan to develop new control schemes, highlighting in this way the limitations of the classical description.

Supervisor: **Dr. Károly Tókési**

PF1/451-20

Investigation of ultrafast processes in intensive laser-material collisions

Recent advances in the generation of well-characterized femtosecond and sub-femtosecond laser pulses have opened up unprecedented opportunities for the real-time observation of electronic dynamics in atoms, molecules and solids. This field has been coined attosecond chronoscopy or, for short, attosecond physics. Such attosecond chronoscopy allows a novel perspective at a wide range of fundamental photophysical and photochemical processes in the time domain. Attosecond chronoscopy raises fundamental conceptual and theoretical questions as to which novel information becomes accessible and which dynamical processes can be controlled and steered. Understanding and describing the tools of interrogation on an attosecond scale is still in its infancy. Recent theoretical developments in this rapidly developing field based on the Monte Carlo technique will be the subject of PhD work. The PhD work will be the development of a program based on classical or quantum mechanics to study the excitation and ionization of atoms and / or molecules (describing the holographic patterns, interpretation and description of photoelectron streaking spectra.)

Requirements: Basic knowledge of atomic physics, quantum and classical physics.

Knowledge of programming language (Fortran, C, C++ etc).

Good skill of manuscript writing in English The recently

Electron-induced reactivity of molecular radicals and cations in non-equilibrium plasmas

Weakly ionized gases containing neutral and charged molecules, electrons, clusters and even solid particles are the components of many non-equilibrium plasmas (NEP). These plasmas are involved in a large variety of processes in novel material production (nanostructures, etc.), optoelectronics, energy storage, fuel gas treatment and fuel conversion. The NEP chemistry, very rich due to the presence of radicals, ions and electrons, results often in large molecular species. This is also strongly relevant for astrophysics [1,2] and in planetary atmospheres [3]. In spite of their heuristic and practical interest, the NEP's are still very poorly understood because of the high complexity and diversity of the phenomena governing them, on scales ranging from microscopic to macroscopic in a very intricate manner. Indeed, simultaneously can take place gas phase collisional processes between electrons and atoms/molecules (electron-heavy collisions) leading to dissociations, excitations and ionizations, collisions between radicals or ions and other molecules (heavy-heavy collisions), plasma-surface interaction processes, nanoparticle growth and dynamics, transport phenomena, collective and dusty plasma effects, etc. Thus, the kinetic modeling of such complex environments requires multiscale physical and numerical models [4] and experimental measurements [5] of the complex elementary processes taking place in the laboratory-generated NEP's.

The present proposal focuses on a limited part of this complexity, namely on the role of electron/molecule collisions in these plasmas. We will restrict ourselves to hydrocarbon (HC)-based plasmas, in which methane (CH_4) and acetylene (C_2H_2) are often the major species. Due to the reactive collisions of the feed gas molecules with the electrons, secondary radicals are formed. These radicals, as experimental findings in diamond deposition suggest, can crucially change the HC plasma characteristics and lead to seriously increased growth rates.

The main question we plan to address in the proposal is: How small secondary radicals produced through the interaction of the HC plasma feed gas with electrons contribute, via attachment/recombination/dissociation processes, to the plasma properties?

This question, as far as we know, have never been considered in a detailed, quantitative manner, and it will be addressed through the investigation of the reaction dynamics between free electrons and the secondary radicals C_2H and CH , as well as their related cations. Thus, quantum approaches, namely Multichannel Quantum Defect Theory [2], R-matrix Theory [6] - all relying on advanced quantum chemistry calculations - will be carried out to investigate the reaction dynamics, to identify the reaction routes and to calculate the corresponding cross sections and rate coefficients.

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II. Nuclear Physics program

Supervisor: **Dr. Julius Csikai**

PF2/42-93

Investigations on fast neutron dosimetry and therapy

A new method developed for the measurement of the volume integrated flux density spectra renders it possible the determination of the neutron doses averaged over the whole body or any organs. For the unfolding of the spectra produced by the primary 14 MeV neutrons, precise dosimetry reactions and improved computer codes are available. Therefore, the doses can be determined for real conditions with high precision by which the different model calculations can be checked. The main goal of these investigations is to measure the dose values averaged over the whole body as well as over the different organs using standard man and standard woman phantom solutions. On the basis of these results, data required by the fast neutron therapy will be determined and the absolute calibration of the dosimeters will be carried out. In addition, the different model calculations are planned to check.

Supervisor: **Dr. József Cseh**

PF2/43-93

Symmetries in nuclei

The group theoretical methods proved to be very efficient in several branches of physics for the description of many-body systems. There are several group theoretical models also in nuclear physics. Based on the concept of symmetries it was possible to systematise and interpret a lot of experimental data, and in addition, the interrelation of several models became more transparent.

Both for the shell model and for the collective model the group theoretical approach turned out to be very important. The third basic nuclear model, the cluster model is being formulated in a purely algebraic language now days. The further development and the application of this technique raises several questions, which can be answered in PhD theses.

These investigations are related to some classical areas of nuclear spectroscopy and reaction studies, as well as to new phenomena, like exotic radioactivity and super (hyper,...) deformations of nuclei.

Beside nuclear physics, there are interesting methodical aspects of this topic, e.g. the use of Hopf algebras in physics, the extension of the concept of dynamical symmetry...

Supervisors: **Dr. Julius Csikai, Dr. Péter Raics, Dr. Ferenc Tárkányi** **PF2/44-93**

Applications of cyclotron neutron source in science and technology

The set up of the MGC-20 cyclotron in Debrecen has opened new possibilities in the determination of microscopic and integral neutron data and the applications of neutrons in technology. These investigations requires precise neutron energies, low energy spreads and to optimise the signal-to-background ratio. It is needed to develop new methods for the measurement of the neutron energy and energy spread as well as for the determination of the

flux density spectra in the case of extended samples. This project could assure a successful international collaboration in the utilisation of cyclotron neutron sources.

The co-workers of the two institutions (KLTE, ATOMKI) have collected experiences at neutron generators, tandem accelerators and various cyclotrons in the production and applications of neutrons which could guarantee a successful research programme in the next years.

Supervisors: **Dr. Julius Csikai, Dr. Sándor Sudár**

PF2/45-93

Investigations on fast neutron induced reactions

During the last 30 years systematic investigations were carried out in Debrecen on the different interactions of fast neutrons with nuclei.

Results achieved could help in the better understanding of the theory of reaction mechanisms and to complete data required by the international data banks. A part of these investigations were carried out in international cooperations (Jülich, Geesthacht, Vienna, Argonne, Obninsk, Kiev) and under the Research Contracts and Agreements with the International Atomic Energy Agency (Vienna). The accelerators and measuring equipment (low voltage neutron generators, MGC-20 cyclotron, gamma- and neutron spectrometers of high resolutions and efficiencies, data processing systems and codes, fast sample transfer technique) available in Debrecen render it possible to complete the neutron data measured by activation and prompt methods. In addition to the measurements of the activation cross sections in a wide energy range, the detection of prompt gammas, neutrons and fission fragments as well as the interpretation of the results will be involved in the programme.

Supervisor: **Dr. Attila Krasznahorkay**

PF2/48-93

Nuclear spectroscopy investigation of the superdeformed states in the actinide region

The discovery of the high-spin superdeformed states at the 80'-es gave a big impetus to the nuclear spectroscopy investigations. The significance of studies of nuclei in the superdeformed state is that the mean field is different from that in normal nuclei: the 2:1 axis ratio means that the surface-to volume ratio is different and the mean field is in some sense stretched and deformed.

In the ATOMKI we are working on a novel approach of this phenomena. The low-spin superdeformed states built on the well-known superdeformed fission isomeric states is going to be investigated. The superdeformed states in actinide region (U, Ac, Np, Pu...) can be excited using (p,p'), (d,p), (^3He ,p) and (α ,p) reactions. The energy of the outgoing protons will be analysed using a split-pole magnetic spectrograph. The excited states built on the fission isomeric states is selected by measuring delayed coincidence of the spectrograph events with the fission fragments.

There are only four rotational bands have been identified with $0^+ \rightarrow 2^+ \rightarrow 4^+ \rightarrow 6^+$ in this region. In this work we are going to search for new excited states, to determine their spins and decay properties to get information for their structure. These new sort of experimental data may help to improve the existing theoretical models.

Phase transitions of nuclear matter

By the variation of the density and/or the temperature of nuclear matter various phase transitions may take place. The study of these phase transitions is important on one hand from the point of view of the understanding of some "natural" systems like the heavy nuclei, the neutron stars, the supernovae, the big bang etc. On the other hand it is needed from the point of view of the explanation of the "artificial" heavy ion reactions. This last topics is rather important and relevant nowadays since there is a chance to produce an up till now unknown phase of matter, namely the quark-gluon plasma. The research going on now and planed for the future is directed for the study of states having a periodic structure. As far as the didactic features are concerned, these topics incorporates the methods of the hydrodynamics, the thermodynamics, the statistical physics, the nuclear physics, the particle physics and the relativistic field theory.

Microscopic description of nuclear systems

It is a commonplace that the constituents of atoms, molecules, solids and nuclei form mean potential fields, and in first approximation, the electrons and the nucleons, respectively, can be considered independent particles moving in these potentials. That is how orbits are brought about, which are organised into shells or bands. But nuclei do as well provide examples defying this rule; there are nuclei, whose constituents, are organised into clusters, which do not support a common mean field and do not build up shells. Such are the light neutron-rich (or proton-rich) nuclei. In these nuclei the nucleons that cannot be admitted into clusters move like clusters themselves. To describe this situation, we say that the system governed by few-body dynamics. The most spectacular phenomena that neutron-rich nuclei produce are neutron halos, which are formed by one or two stray neutrons, kept on extremely loose leash. At present the investigation of these nuclei seems to be the hottest issue in nuclear structure physics.

With Japanese partners we have developed a method to describe bound state systems showing few-body dynamics. We have applied this method in neutron-halo nuclei, to few-nucleon systems, radioactive decay with cluster emission, to molecules, to mesonic molecules, to electron-positron systems, to hadrons as multiquark systems, to irregularities of solids so called excitons and to localised few-electron systems on semiconductor samples called quantum dots. Open problems remain in all these fields, and there are various international partnerships in which these fields are being investigated.

A student could join in this work at several points. The work on these projects requires the knowledge of elementary quantum mechanics. Since most of the voluminous calculations are analytical, which is very rare in modern physics, it requires some affinity to, and working skill in manipulating mathematical formulae. The student will have an opportunity to master not only numerical computation but algebraic computation as well. As an outcome, the student will get familiar with the principles of the construction of physical models, with the relevant branch of physics (e. g., in nuclear structure physics), and will get considerable practice in computing.

Study of the structure of medium-heavy nuclei in heavy-ion reactions

In the nuclear structure research based on heavy-ion induced reactions the study of high-spin nuclear states has become of more importance since the 1980's, which can be ascribed to bringing the sophisticated gamma-ray detector systems into use. The increase of detection efficiency of these systems has then enabled not only the extension of studying excited nuclear states towards even higher energies and spins, but the study of very low cross section nuclear processes, as well. Such investigations led e.g. to the discovery of high-spin superdeformed states and later on to the systematic study of the (highly elongated) superdeformed nuclei; to the simultaneous observation of different nuclear shapes in a given spin range (shape co-existence); or to the observation of band terminations, which is caused by a shape change as the excitation energy is increasing along a rotational band. We have participated in such investigations since the early 80's, in the framework of international collaborations. At present our experiments are based on the EUROBALL detector system developed in collaboration by many Western-European countries. In order to extend the study of extreme nuclear states into nuclear mass regions not accessible by stable beams, we have started to use recently the newly available radioactive beams. Related to this new direction of gamma-spectroscopy we participate in the development of the EXOGAM detector system to be operational at the GANIL facility, France.

The task of the candidate(s) for this Ph.D. program would be to participate either in the study of the extreme deformations of nuclei in the indicated mass regions (**PF2/413a-93**) or in the study of band terminations of some $A \gg 100$ nuclei (**PF2/413b-93**). The candidate is expected to play an important role in the analysis of the already available data or the data to be collected with his/her participation, and also in the interpretation and publication of the results. In the first program, experiments will be carried out in France within an English-French-Hungarian collaboration using the EUROBALL and the EXOGAM detector systems. The experiment planned within the second program will most probably be carried out with the GAMMASPHERE detector system. Data evaluation will be done in both cases using the data analysis software installed on the UNIX workstations available at our institute (the Institute of Nuclear Research).

PF2/413a-93**Study of the structure of medium-heavy nuclei in heavy-ion reactions;
Extreme nuclear deformations**

The main goal of this research program is the study of extreme nuclear deformations in some $A \gg 130, 150$ and $A \gg 170$ nuclei. The superdeformed and hyperdeformed nuclei are meant here as having extreme deformations. At these deformations the nucleus has elongated shape of 2:1 and 3:1 axis ratios, respectively, which are related to the second and third minimum in the potential energy surface of the nucleus. These extreme nuclear deformations are manifested by rotational bands which, in a wide spin region, resemble the rotational spectra of ideal rigid rotors having such deformations. Even today, in most of the superdeformed nuclei, the deexcitation of the superdeformed states to the normal deformed states is not known, consequently the excitation energy and spin of the corresponding

collective states are undetermined. Another interesting subject worth studying is the appearance of twin superdeformed bands which show very similar transition energies in some neighbouring nuclei. On the basis of theoretical predictions, the formation of hyperdeformed nuclear states is expected at even higher spins (consequently at even smaller cross sections) than superdeformed states, and most probably in correlation with the emission of charged particles. Accordingly, their observation using gamma-spectroscopy techniques is thought to be successful only when the present gamma-detector systems are used together with ancillary detectors aiming at the selective detection of light charged particles. At present we participate in research which aims at the identification of hyperdeformed states in some $A \gg 150$ and $A \gg 170$ nuclei, using nuclear reactions associated with charged-particle emission and an ancillary detector system developed in the ATOMKI for EUROBALL.

PF2/413b-93

Study of the structure of medium-heavy nuclei in heavy-ion reactions; Shape changes in nuclei

Another research field of us is the study of nuclear shape changes with increasing excitation energy. The manifestation of shape change could be the termination of collective bands, when the nucleus consecutively changes its elongated shape favouring collective excitations into a near-oblate (or spherical) shape favouring single-particle excitations. In this sphere-like shape the nuclear spin is built up solely from the spin contribution of the individual nucleons, therefore for a given nucleon configuration this spin has a maximum value at which spin the collective band terminates (the terminating spin). From a recent experiment using similar experimental techniques as mentioned in connection with the first subject, such terminating bands have been observed in several $A \gg 100$ Ru, Rh and Pd nuclei. The configuration of each bands has been identified and a systematic behaviour has been found concerning the structure of the bands belonging to different configurations. The change of deformation along terminating bands can be demonstrated in a direct way by measuring the lifetimes of the corresponding levels. An experiment aiming at the determination of the extent of shape change in these nuclei is planned as part of the PhD program, using either the GAMMASPHERE (USA) or the GASP (Italy) detector systems.

Supervisors: **Dr. Julius Csikai**

PF2/414-93

Chemical Analytical Applications Based on Prompt-Gamma Radiation

The data on fast neutron induced prompt-gamma radiations are rather scarce even according to the latest evaluations of nuclear data centres. The recent development of gamma spectrometry and data handling renders it possible to study systematically this type of complex gamma spectra needed for practical purposes, like shielding design, as well as for detailed studies for nuclear reaction mechanism.

The elaboration of this method opens new possibilities to utilise the low voltage neutron generators and provides access to the more complex experimental facilities with wide range of neutron energy.

The immediate basic aim of this theme the determination and interpretation of partial cross sections belonging to the excited states of residual nucleus induced in $(n,2n)$ reactions as well as completion of σ_{prod} production cross sections for practical applications.

Supervisors: **Dr. Ferenc Tárkányi**

PF2/418a-b-93

Investigation of cross sections of charged particle induced nuclear reactions

Determination of cross section of nuclear reactions play an important role for investigation of mechanism of nuclear reactions and in optimisation of different application of nuclear reactions in practice. The topic investigated is closely related to the following two sub-topics:

PF2/418a-93

Investigation of cross sections of charged particle induced nuclear reactions for basic science

Cross section ratios of long lived isomeric states having different spins gives information on the distribution of spins of level densities of product nuclei and on reaction mechanism. Systematical investigations on broad range of nuclei using different bombarding particles have special importance. The measurements will be done on the beams of the Debrecen MGC cyclotron by activation technique. For interpretation of the data different model codes will be used.

PF2/418b-93

Investigation of cross sections of charged particle induced nuclear reactions for application in practice

The application of accelerators is based mainly on charged particle induced nuclear reactions. Knowledge of cross sections play important role in isotope production, wear measurement using thin layer activation technique, and activation analysis and on other applied fields. The application connected investigations will deal with the measurements of new or contradicting nuclear data and with critical comparison of theoretical and experimental values. The measuring technique and the data evaluation are similar as described above.

Both sub-topic contains experimental and theoretical tasks.

Supervisor: **Dr. Tamás Vertse**

PF2/419-94

Calculation of the continuum in spherical and deformed potentials using complex scaling

In certain quantum mechanical problems it is an efficient way of taking the effect of the continuous spectra of a Hamiltonian (continuum) into account by separating the resonant part of the continuum from the smooth background. Resonances can be considered as complex energy eigenstates of the Hamiltonian with eigenfunctions having diverging asymptotics. Complex scaling is a method for regularising integrals of the diverging wave functions. The effect of the non resonant part of the continuum can either be neglected or taken into account by using scattering states of a complex path. The aim of this project is the

application of this method for the mean field used in nuclear physics, e.g. spherical and deformed shell model potentials (with finite depth) or the complex optical potential. The task is as follows:

- To determine the energies and wave functions belonging to the resonances by integrating the radial or coupled Schrödinger equations numerically.
- To determine the scattering states with complex energies in the potentials mentioned.
- To calculate the expectation values of different physical quantities using a basis composed of bound resonant and scattering states.
- To check the accuracy of the approach in the case of model potentials.

Supervisor: **Dr. Julius Csikai**

PF2/424-95

Determinations of differential and integral neutron data for applications

There are about 150 different instrumental techniques and methods used in elemental analysis. The applications of neutrons have the following main advantages: fast and non destructive, no matrix problems especially for fast neutrons, multielemental analysis of complex samples is possible, applicable for small and bulk samples using sampling, in-situ and on-stream procedures. Isotope neutron sources such as about 5 Ci ($\sim 7 \times 10^6$ n/s) of Pu-Be, Am-Be or a few hundred micrograms ($\sim 7 \times 10^8$ n/s) of ^{252}Cf and small neutron generators ($\sim 10^{11}$ n/s) based on the $^3\text{H}(d,n)^4\text{He}$ reaction are applicable for materials research via the activation and nuclear reaction analyses, as well as by using the neutron reflection and transmission methods. The high penetrating ability of neutrons and gamma-rays renders possible the multielemental analysis of bulk (\gg kg) samples. The prompt gamma-rays emitted in thermal neutron capture (n,γ), inelastic scattering ($n,n'\gamma$) and fast neutron induced reactions ($n,x\gamma$) are widely used in elemental analysis of geological samples, nuclear and chemical explosives, illicit drugs and other contraband materials. In addition, the neutron induced reactions producing radioisotopes are also commonly used in the elemental analysis and in the study of irradiation effects in solids and biological samples.

The sensitivity and accuracy of the neutron based analytical methods depend on the optimal flux density ratio of the primary fast and thermal neutrons. Therefore, the flux density distributions of thermal and primary 14 MeV neutrons must be measured in different geometrical configurations of bulk samples. Analytical expressions are required for the calculations of the absolute flux values of neutrons in various moderator-sample-reflector geometries. Attenuation characteristics of different samples must be determined for ^{252}Cf , Pu-Be and 14 MeV neutrons. Relative fractions of neutrons above the ($n,n'\gamma$) and ($n,x\gamma$) reaction thresholds for various isotopes vs. sample thickness should be determined. On the basis of the cross section curves of ($n,n'\gamma$) and (n,x) reactions and the flux density spectra measured for different sample thicknesses the dependence of reaction rates, $R(E_n)$, must be calculated for different elements and isotopes. The energy integrated reaction rates as a function of sample thickness should also be determined and the obtained analytical expressions are required to be interpreted. In such cases where the cross section curves are not well known new measurements are needed. The measurements of the spectrum averaged cross sections can also be used for testing the recommended excitation functions.

Investigation of charged particle detectors used for nuclear physics experiments

For the investigation of the high spin states of nuclei (e.g. those of the superdeformed ones) sophisticated multidetector systems are used. These are mainly gamma detectors consisting of large volume high purity germanium detectors (e.g. the EUROGAM and EUROBALL systems), but for the identification of the reaction channels ancillary particle detectors are also used by determining the type, the energy and the angular distribution of the particles.

Different kind of detectors can be used as particle detector: semiconductor detector, scintillation detector or the combination of these. For this purpose CsI(Tl) scintillation crystals combined with PIN photodiodes are widely used nowadays.

During the elaboration of the present topic the candidate's task is the investigation of two types of detectors. One of them is the scintillation detector consisting of CsI(Tl) crystal and PIN photodiode and the other one is the combination of this detector with Si semiconductor detector of surface barrier type. The purpose of the investigations is the optimization of the detector parameters and the comparison of the relative advantages of these two types of detectors.

During the processing of the detector signal the aim is to gain the maximum available information from the signal and to reach a particle discrimination threshold as a function of the particle energy as low as possible. This can be achieved by choosing the best particle discrimination method and by the optimization of the discrimination technique applied.

The electronics of the EUROBALL gamma detector system is built in VXI system, which is very effective for multichannel applications. For compatibility reasons it is expedient to build the electronic part of the ancillary detectors also in VXI. Therefore it is an essential part of this topic to get acquainted with and be able to apply the VXI system.

Potential problems of quantum mechanics and their applications

Models based on various potentials proved to be essential in the description of subatomic phenomena. These problems are usually solved using numerical methods, nevertheless, analytical solutions are also possible for certain model problems. The study of these latter cases is important in many respects:

1. Exactly solvable problems can help the development of numerical techniques, as they can be used for testing purposes, and can also be combined directly with the numerical methods.
2. In the past decade new methods have been introduced by which the simplest model potentials can be generalized, and therefore exact solutions can be given for more extensive classes of potentials which can be better adapted to realistic applications.
3. The potential based description can be extended towards systems of coupled degrees of freedom (spins, multichannel systems, etc.) and exactly solvable problems can be developed in these cases as well.

Among the possible applications of these methods we mention problems related to the screened Coulomb potentials, atoms in electromagnetic fields, optical potentials, resonance phenomena, etc.

Supervisor: **Dr. Julius Csikai**

PF2/429-97

Bulk media assay by neutrons and gamma-rays

The high penetrating ability of neutrons and gamma rays renders possible the multi-elemental analyses of bulk ($M \gg \text{kg}$), ($V \gg \text{m}^3$) samples. Pulsed fast neutron analysis, associated particle imaging and pulsed fast-thermal neutron analysis can determine the concentration and location of different elements in extended samples.

Some typical fields:

1. Geological materials. On line analysis is required e. g. by coal mines, coal preparation plants, coal fired power plants. Concentrations of H, C, O, and N give information on calorific value, S on environmental pollution, Cl on corrosion of boiler, Si, Ca and Fe on ash content.
2. Detection of illicit drugs and other contraband materials in cargo containers. Nuclear interrogation techniques based on fast neutrons have the potential for identifying H, C, N, O, Cl as constituent elements of illicit drugs. Separation between target materials and surrounding benign background materials needs to measure the concentration of these elements and their ratios.
3. Chemical explosives. The concentrations of light elements and their atomic ratios (C/O, C/N, O/N, H/C) render possible the detection of explosives. Nuclear techniques based on neutrons from isotope or small accelerator sources are successfully used for detection of explosives in airline luggage (suitcases, briefcases, small boxes).

Methods in large (8'x8'x20') unopened cargo containers require further investigations in the fields of the determination of flux density spectra of neutrons and the characteristic parameters of their interactions.

Supervisor: **Dr. Julius Csikai**

PF2/430-01

Application of nuclear methods for identification of illicit materials

(see PF2/429-97)

Supervisor: **Dr. Attila Krasznahorkay**

PF2/431-02

Study of giant resonances and measurement of neutron-skin thicknesses in radioactive beams

One of the most important direction of our contemporary nuclear structure research is the usage of radioactive beams. These programs have been started already in Germany at GSI, in France at GANIL, in the USA at NSCL and also in Japan at RIKEN. The nuclear spectroscopy section of ATOMKI started fruitful collaborations with the mentioned laboratories during the last few years. The main reason of this increased interest is the possibility to study the large „Terra incognita” in the nuclear landscape. Of the 7000 particle-stable isotopes, only 263 stable are found in the nature, and only about 2000 could be studied

up till now. The present models for nuclear structure, dynamics and evolution are unlikely to survive intact in this expanded horizon.

Nuclear properties, which can not be observed in nuclei near the stability line have already been revealed. One of them is the neutron halo, and another one is the neutron skin in neutron-rich nuclei, when the neutron matter covers the nucleus like a skin. The neutron halo and neutron skin effect the structure of the nucleus both in their ground state and in their excited states.

By measuring the thickness of the neutron skin one may constrain the symmetry energy term of the nuclear interaction, which is essential not only for describing the structure of neutron-rich nuclei, but also for describing the properties of the neutron-rich matter for e.g. for calculating the size of a neutron star. In our previous works we have demonstrated that the cross section of the spin dipole resonance (SDR) is unambiguously related to the neutron-skin thickness. During the PhD scholarship, we would like to study the giant resonances and use this effect to measure the neutron-skin thickness for a wide range of isotopes. My experimental proposal of „Experimental study of neutron-skin thicknesses in neutron-rich isotopes of $28 \leq Z \leq 50$ ” has been accepted at GSI. We are planning to start the experiments in 2002.

Supervisor: **Dr. Endre Somorjai**

PF2/432-02

Experimental study of astrophysical p-process.

The nucleosynthesis of the isotopes above the iron region proceeds mostly through series of neutron capture reactions, called s- and r- processes. For tens of years detailed investigations of these reactions have been done and the experimental results reproduce the abundances of the s- and r-isotopes. However, a small part of the proton-rich heavy isotopes (p-nuclei) cannot be produced by the above mentioned processes, for their synthesis should exist some other, secondary process (p-process) corresponding to their very low natural abundances. According to the presently accepted model, the p-nuclei are synthesized in pre-supernova state or in supernova explosion by successive (g,n) reaction on s- and r- seed nuclei towards proton-rich isotopes. Above a certain neutron deficit, neutron emission is energetically not favoured, the (g,p) and (g, α) reactions are preferred and their cross section determines the abundance of the p/nuclei. One of the major problems is the lack of the experimental data, hence the input for the calculation of the reaction chain is purely based on Hauser-Feshbach statistical model.

The experimental investigation is possible through the study of the inverse reactions, i.e. (p,g) and (α ,g) reactions at astrophysically relevant energies lying far below the Coulomb barrier. At these energies the reaction cross sections are very low which explains the scarcity of experimental data. In the last few years a specific experimental method has been developed in the ATOMKI for the study of the low cross sections of the (p,g) and (α ,g) reactions. To perform that kind of experiments is the task of the PhD student.

Teaching Nuclear Physics in Secondary School

Final program may be completed after discussing candidate's abilities, education experiences in nuclear physics, traditions and possibilities of his/her school. All research topics must contain experiment, demonstration and/or evaluation, data processing. Elaboration of the thesis may exploit the potential of the nuclear research facilities in Debrecen as well as in Budapest and Paks. Teachers should be familiar with these laboratories being the main targets for school excursions, too.

Nuclear transmutations and their importance in energetics

Radioactive decay law in experiments and applications. Characteristics of α -, β - and γ -decay and their relations to nuclear structure. Nuclear reactions. Neutron physics. Energy release and nuclear characteristics. Energy production by fission and fusion. Operation and safety of nuclear power plants. Creation of education materials for web-site regarding the importance and environmental effects of nuclear energy. Development of student experiments, demonstration tools and teaching methods to deepen ideas of nuclear physics phenomena. Foundation of data bases supporting students' individual study. Investigation of applications in nuclear analytical techniques.

Interaction of radiations with matter

Energy loss and range of charged particles. Penetration of γ -radiation through matter. Detectors: photo-emulsion, solid-state nuclear track detector, cloud chamber, GM-counter. Scintillation and semiconductor spectrometers. Radiation protection and dosimetry. Natural radioactivity and environmental effects. Demonstrations in nuclear physics. Assembling experiments and measurements to be performed in secondary schools. Planning study circle activities. Production of teaching materials supporting students' individual study. Production of teaching materials on radiation defects and radiation protection. Presentation and analysis of applications by video films.

Astronomy in the Teaching Physics (The use of Nuclear Physics)

1. Subthemes
 - 1.1. Relation between Physics and Astronomy in a historical approach
 - 1.2. Star formation and nuclear physics
2. Tasks

- 2.1. Scientific basis of the school subject: Astronomy Computer simulations: formation of stars, Hertzsprung-Russell diagram, nuclear reactions, nuclear energy, energy production of stars, origin of the chemical elements)
 - 2.2. Teaching astronomy at the schools recently. The place of the astronomy and the nuclear physics in the whole teaching physics, connections between the school subjects.
 - 2.3. Methods of the teaching modern Astronomy – why, what and how?
 - 2.4. Evaluating some parts of the enlarged texts of the secondary school-astronomy.
- Suggestions for all educational level
- the role of gravitation on the Earth, in the Solarsystem, in the galaxy
 - motion near the Earth
 - motion of the satellites, planets
 - weightlessness
 - solar and moon eclipse
 - evaluation of stars, origin of planets
- 2.5. Visual aids: demonstrations, demonstrational experiments, using www
 - 2.6. Making a CD-ROM and its use at the school
 - 2.7. International investigations in the schools (France, Russia)
 - 2.8. Plans for the future investigations in the field of teaching astronomy based on nuclear physics (teaching experiments, tests)

Supervisor: **Dr. Zsolt Fülöp**

PF2/436-06

Studies in nuclear astrophysics

We investigate experimentally the nuclear physics aspects of stars and supernovae. Nuclear reactions are responsible for the energy generation of stellar objects as well as for the creation of elements through nucleosynthesis in static and explosive stellar scenarios. The experiments involve mainly cross section determinations and relevant nuclear data studies using a wide range of particle accelerators worldwide. Although nuclear astrophysics has been studied for many years, the direct study of the astrophysical reactions is extremely difficult, since in static scenarios the cross sections are extremely low, and in explosive scenarios rare/radioactive nuclei are involved. For ultra-low cross sections the natural background can hamper the yields to be measured, therefore we can use the unique underground laboratory, LNGS, Gran Sasso, Italy. Since we are members of the LUNA (Laboratory for Underground Nuclear Astrophysics) collaboration, the access to this facility is granted. Our experiments will provide answer on so far unsolved puzzles of the creation of elements.

Supervisor: **Dr. Zsolt Fülöp**

PF2/437-06

Studies in exotic nuclear physics

Very neutron-rich light nuclei will be studied in this topic, which requires intense radioisotope (RI) beams, new experimental methods and sensitive detection devices because of the low reaction cross sections. We intend to use fast RI beams available at RIKEN Accelerator Research Facility to investigate two typical anomalous phenomena of unstable

nuclei by coupling the in-beam gamma-ray spectroscopy method and direct nuclear reactions suitable for the beam conditions:

- i) decoupling of the proton and neutron motion in nuclei,
- ii) disappearance of neutron magic numbers.

Supervisor: **Dr. János Timár** and **Dr. Dorottya Kunné Sohler**

PF2/438-06

Interaction between collective and individual motions in rotating nuclei

The rotation of nuclei allows investigation of a special type of the quantum mechanical rotation, where the interaction of the rotation with other excitation modes provides special phenomena, that cannot occur in other quantum mechanical systems. Such phenomena are for example the chiral symmetry breaking, the termination of rotational bands or the anomalous signature splitting of dipole rotational bands, as well as appearance of super- and hyperdeformed nuclear shapes. Studies on such phenomena gives a main part of the planned research topic. A necessary condition of the quantum mechanical rotation is that the rotating object should have a non-spherical (deformed) shape. Deformed nuclear shapes can be found in the regions far from shell closures. These regions are known close to the stability line, but not well known far from the stability line. Mapping of new regions far from the stability line is going on currently mainly using radioactive beams. Such studies give the other main part of the planned research topic.

Supervisor: **Dr. Kornél Sailer, Dr. Sándor Nagy**

PF2/439-07

Non-locality in quantum mechanics in quantum field-theoric terms

One of the basic features of the states in quantum mechanics is their non-locality. The recent experimental results obtained on entangled states show up the presence of correlations among observations at spacetime points with spacelike separation. This is supported also by the recent results of the so-called delayed choice interference experiment proposed by Wheeler. Therefore a paradoxical situation has been arisen between quantum mechanics and the theory of special relativity, namely it seems that information might propagate faster than the speed of light in the vacuum. The experiments performed for the demonstration of quantum mechanical non-locality have generally been explained in terms of quantum mechanics and relativistic considerations introduced afterwards in heuristic manner.

The task is first, to overview the results of the experiments performed for the demonstration of quantum mechanical non-locality, secondly to develop the quantum field theoretic method for the description of simple quantum mechanical interference experiments, and finally to show that the problem of non-locality stands even in a truly relativistic quantum field theoretic description.

Supervisor: **Dr. Julius Csikai**

PF2/440-08

Determinations of hydrogen content and the C/H atomic ratio in bulk samples using neutrons.

The International Atomic Energy Agency has organized a coordinated research program in 1997 on „Bulk Hydrogen Analysis using Neutrons”. The scientific scope of the project is to determinations of hydrogen content and the C/H atomic ratio in minerals, agricultural- and industrial products, coal and oil samples, as well as in plastic explosives. In the frame of the project the UD Institute of Experimental Physics has dealt with the following topics and intend to continue in the future, too: 1) Determination of hydrogen by thermal neutron reflection method. 2) Determination of hydrogen by slowing down of epithermal neutrons. 3) Determination of hydrogen by the measurements and MCNP calculations of leakage spectra of neutrons. 4) Investigation of migration of hydrogen in solid states.

Supervisor: **Dr. Julius Csikai**

PF2/441-08

Measurements of leakage neutron spectra and reaction cross-sections.

The main aim of the project to produce new and precise data for accelerator based of transmutation of radioactive waste, for the designing and construction of spallation neutron sources and fusion reactors as well as for reaction model calculations. Excitation functions of neutron induced reactions are scarce and discrepant especially for the production of short-lived isotopes in the 8-12 MeV incident energy range. These investigations can be carried out by using the fast sample transfer system at the MGC-20 cyclotron of ATOMKI as well as the Pulse Height Response Spectrometry based on a NE213 scintillator. Method for the measurements of activation cross-sections has been developed and applied routinely. Transport experiments have been started for Bi and Pb targets using broad spectrum of d+Be reaction as well as monoenergetic D+D neutrons. These investigations are in progress.

Supervisor: **Dr. Zsolt Schram**

PF2/442-08

Thermodynamics in non-abelian lattice gauge theories

In high energy heavy-ion collisions formation of a new phase of matter, the quark-gluon plasma is expected. For non-abelian gauge fields calculations based on the grand canonical ensemble showed the existence of a deconfining phase transition at finite temperature. However, clearly the application of the grand canonical ensemble at zero baryon density is a strong simplification. Calculations at finite baryon density has been done recently, but these are difficult and there are still a number of questions to answer. In our work we carry out lattice studies in various gauge theories using a new method where, instead of the usual (grand) canonical distribution, we implement in the simulations the so-called Tsallis distribution which shows power-like characteristics at higher energies. This novel approach can be formally interpreted as calculating expectation values of observables over fluctuating temperature. In our case the temperature fluctuates with a Gamma distribution. Our aim is to explore the phase structure of the systems under consideration and to determine the corresponding equations of state.

Supervisor: **Dr. Rezső Lovas**

PF2/443-08

Nuclear fission with swift fragments

In a fission process the liquid drop of an atomic nucleus is made elongated by the Coulomb repulsion, its neck gets cut and the fission products are tossed apart. The emission of neutrons can be neglected since the dynamics of the process is hardly influenced by them. Semiclassically, the process can be described as the evolution of a single parameter, which can be chosen to be the distance s between the two mean-field potentials representing the fragments.

The total energy E of the system as a function of s [$E(s)$] has a minimum at small values of s , *has a maximum at a larger value, and* decreases monotonically beyond. The function $E(s)$ can be regarded as a potential energy, and, with that, a Schrödinger equation is obtained for the variable s . Its solutions are states reminiscent to bound states within the barrier, but, because of the finite size of the barrier, the binding is not perfect: the states can decay via tunnelling, i.e., the nucleus fissions. In such a model the life times of fissioning states can be predicted very well, and it is physically reasonable to identify the excited states with those found experimentally (e.g., with the famous hyperdeformed states found in Atomki).

Unfortunately, however, $E(s)$ is not a proper potential since the distance s is not an observable in the quantum mechanical sense. Indeed, $E(s)$ contains a sizeable contribution from the nucleonic kinetic energy, which is positive, and that is why it is much shallower than the realistic nucleus-nucleus potentials (which depend on the distance r between the centres of mass of the fragments, rather than on s). In the model with the shallow potentials the swift motion in the deep potential is replaced by a lazy motion. Therefore, the shallow potentials are imperfect for the description of the collision of two nuclei as well.

The objective of the study proposed is to compare the models with the deep and shallow potentials and to understand how the shallow-potential model seems to work well in spite of its conceptual defect. The two potentials are related to each other through an integral transformation. In a model in which the fragment wave functions are expressed in terms of harmonic-oscillator single-particle states, the transformation can be performed exactly or approximately. To my best knowledge, the deep-potential model has not yet been used for nuclear fission.

A candidate should have a basic knowledge of quantum mechanics and should be able to treat quantum mechanical formulae both analytically and numerically. He/she will have an opportunity to apply symbolic computing as well.

Supervisor: **Dr. Péter Raics**

PF2/444-08

Teaching nuclear physics in secondary school

Theses are offered to teachers in secondary schools and college in different eligible sub topics.

Purpose: education of fundamental phenomena in nuclear physics and its applications; realistic concepts of radioactivity, nuclear physics.

Method: demonstrations, experiments; sample examples, tasks for calculations; audio-visual problems and solutions, e-education, audio-visual methods, construction of web-sites.

Natural and artificial radioactivity. Application of simple radioactivity detectors. Demonstrations with a diffusion cloud chamber. Determination of half-life; investigation of nuclide chains. Radioactivity in the environment.

Interaction of radiations with matter. Charged particles, neutrons and gamma-photons. Detection and spectrometry and their utilization. Cloud chamber in alpha-spectrometry. Dosimetry and radiation protection. Radon-problem.

Nuclear reactions and their significance in nuclear energy production. Investigation of radioactive decays and simple nuclear processes with cloud chamber, GM-tube, scintillation and semiconductor detectors. Explanation of benefits and disadvantages of nuclear energy production. Effects in the environment.

Supervisor: **Dr. József Molnár**

PF2/445-08

Digital processing of detector signals applied in nuclear medicine and in nuclear physics

Digital signal processing (DSP) is the study of [signals](#) in a [digital](#) representation and the processing methods of these signals. DSP includes subfields like: [audio](#) and [speech signal processing](#), sonar and radar signal processing, sensor array processing, spectral estimation, statistical signal processing, [image processing](#), signal processing for communications, biomedical signal processing, seismic data processing, etc. DSP [algorithms](#) have traditionally run on specialized processors called [digital signal processors](#) (DSPs). Algorithms requiring more performance than DSPs could provide were typically implemented using [application-specific integrated circuit](#) (ASICs). Today however there are a number of technologies used for digital signal processing. These include more powerful general purpose [microprocessors](#), [field-programmable gate arrays](#) (FPGAs), [digital signal controllers](#) (mostly for industrial apps such as motor control), and [stream processors](#), among others.

Supervisor: **Dr. Attila Krasznahorkay**

PF2/446-08

Probing a light neutral boson in internal pair creation

In a recent series of papers the intriguing possibility was explored that the cosmic dark matter consists of new elementary particles with masses in the MeV range, which could be searched for in nuclear physics laboratories. In order to study the possible signatures of the above particle, we are planning to design and build a Compact Orange type Positron Electron spectrometer (COPE) for precise studies of the e^+e^- pair creation in the energy range of 10-20 MeV with large solid angle [UTF-8?]($>2\pi$), good energy (1%) and angular (2°) resolutions using strong permanent magnets. With the presently available tracking detectors, data-acquisition systems and computers we could study the differential internal pair creation process more precisely than ever before, and could search for the effects of the predicted light neutral particles.

Supervisor: **Dr. András Kruppa**

PF2/447-08

Symbolic and numerical computational methods of few body problems of quantum mechanics

The solution of three body problems requires a lot of symbolic and numerical calculations. During the application of the stochastics variational method it is worthwhile to calculate the matrix elements in analytical form. Using the symbolic language Mathematica this task can be simplified. The scattering solution of three charged particles is very

problematic both theoretically and numerically. The complex scaling method may overcome the difficulties.

Supervisor: **Dr. Dorottya Kunné Sohler**

PF2/448-09

Nuclear structure studies by gamma-spectroscopic methods

The nucleus in an excited state decays to the ground state among others by gamma-ray emission. The characteristics of the gamma rays, e.g. their energy, relative intensity, multipolarity and coincidence relations, can be determined by analysing experimental data using gamma-spectroscopic techniques. With the help of the information obtained, the energy and the quantummechanical properties (spin and parity) of the excited states can be deduced and eventually conclusions can be drawn on their configuration.

We intend to study special motions in normal deformed nuclei lying close to the stability line. This can be achieved by measuring the gamma rays emitted by these excitations arising with very low cross sections. Another aim of our research is to investigate the structure of the excited states in drip-line nuclei having extrem proton/neutron ratio, analysing experimental data obtained by using new generation radioactive beam facilities. Both tasks belong to the most up-to-date directions of the contemporary nuclear structure research.

Supervisor: **Dr. Zsolt Fülöp**

PF2/449-10

Study of the life time of radioactive nuclei

Supervisor: **Dr. József Molnár**

PF2/450-10

Development of Position Sensitive Detector Systems with Digital Signal Processing Electronics for Nuclear Physics and Medical Imaging

These developments in international co-operation aim at updating the detectors and signal processing electronics of the charged particle detector system called DIAMANT, furthermore, developing a new gamma detector system called PARIS. Both projects are related to the nuclear physics research planned at SPIRAL-2, a high current accelerator in GANIL (Caen, France) where the EXOGAM2 and PARIS gamma detector systems are planned to be used.

Besides nuclear physics applications, we work with different position sensitive systems for medical and industrial imaging. These developments exploit the advantages of semiconductor based photo detectors (Si Photo Multiplier – SiPM, Avalanche Photo Diode - APD).

The PhD student should construct and test the prototypes of detectors. He is to develop the digital signal processing electronics of the detector systems and work out algorithms to be implemented in programmable logic circuits (FPGA).

Nuclear structure studies by use of radioactive beams

In the last few years the use of radioactive beams in nuclear structure studies became dominant. New radio active beam facilities has been constructed like the SPIRAL in GANIL France, or the RI Beam Factory in RIKEN Japan, or are under construction like the FAIR in GSI Germany or the FRIB facility in MSU, USA. These accelerator centers make possible the reach of new nuclear regions and observation of new nuclear physics phenomena.

The proposed research topic is the study of the structure of nuclei with a proton to neutron ration significantly different from 1:1 by use of in-beam gamma ray spectroscopy. We are going to study the gamma rays from nuclear reactions induced by ions from radioactive beam facilities and to deduce conclusion on the reaction process from the properties of the gamma rays observed.

The experiments will be done in the best international laboratories like RIKEN RIBF, GANIL or GSI. The data processing will be done in ATOMKI, Hungary. The PhD student, in addition to the preparation and performance of the experiments and analysis of the data will have an opportunity to participate in software and detector development related to the experiments.

Functional renormalization group for open quantum systems

The main goal is to study nonequilibrium physics of simple, open quantum systems in quantum field-theoretic framework. It can be investigated the decoherence of a coherent superposition of quantum states due to the influence of environmental effects, the possibility of a phase transition with varying strength to the environment or the temperature of the environment, and open quantum systems showing up dissipative quantum chaos.

There are a lot of important, experimentally realizable simple quantum systems which can be modelled by quantum Brownian motion: a particle moving under the exertion of an external force and coupled to the environment. Following Caldeira and Leggett the environment can be reliably modelled by either a zero-temperature or a finite temperature system of an infinite set of independent harmonic oscillators. The functional renormalization group method enables one, on the one hand to treat the nonperturbative behaviour of the particle moving under the exertion of the external force (e.g. that of the anharmonic oscillator) and, on the other hand, to study the case of strong coupling of the particle to the environment. The model outlined above offers the possibility to investigate the transition from quantum to classical physics. Aiming this one has the possibility to study the effect of the thermal and quantum fluctuations on the decoherence. The systematic treatment of any fluctuations can be performed by the functional renormalization group method. With varying coupling to and temperature of the environment one expects that a new, broken symmetric phase appears in the model. We assume that there is an infrared fixed point in this phase, where the scaling properties of the model change. The fixed point enables us to determine the flow of the couplings around the singularity. We intend to study the phases of the model, and their critical exponents. This requires the inclusion of the wave function renormalization, which can be taken into account self-consistently in the framework of RG method.

Study of nuclear reactions relevant for the synthesis of heavy elements

The astrophysical p-process is the stellar production mechanism of the heavy, proton-rich isotopes. According to our present understanding, the p-process takes place in massive stars towards the end of their evolution, most likely in supernova explosions. The p-process is one of the least known processes of nucleosynthesis, the models are not able to reproduce well the p-isotope abundances observed in nature.

One reason for this problem can be the insufficient knowledge of the nuclear physics input used in p-process models. The models involve a huge network of nuclear reaction, the cross section of the reactions are usually taken from theoretical calculations. The experimental check of the calculated cross section is of crucial importance in order to make the p-process models more reliable.

The main task of the Ph.D. work will be to carry out cross section measurement of charged particle induced [mainly (a,g) és (p,g)] reactions in the mass and energy range relevant for the p-process. The experiments will mainly be carried out using the accelerators of ATOMKI, some measurements, however, will take place in foreign institutions in the framework of international collaborations.

Experimental study of exotic nuclei

Experimental studies with radioactive ion beam are nowadays in the forefront of nuclear physics. The goal of these experiments is to study the structure of atomic nuclei in extreme conditions when the ratio of protons and neutron in the nucleus is very different from that of nuclei in the valley of stability. The topic of the present research is to investigate the change of the magic numbers and the proton-neutron correlation in these exotic, unstable nuclei. However, the intensity of the radioactive ion beams is usually quite low therefore many instruments are required to gain the most pieces of information from an experiment, i.e., all the possible radiation and particles from the nuclear reaction in question are supposed to be detected. Thus, our aim is also to build devices suitable for these experiments, which is part of the present research topic. The experiments are to be performed in large, international collaborations in the following research institutes: RIKEN (Japan), GSI (Germany), GANIL (France).

Experimental study of astrophysically relevant radiative capture reactions

The aim of experimental nuclear astrophysics is to study those nuclear reactions that take place in stars and contribute to the energy generation or nucleosynthesis processes. The nuclear astrophysics group of Atomki carries out research at various subfields of this discipline. Our main research topics comprise the study of the p-process of heavy element nucleosynthesis as well as the investigation of some key reactions of hydrogen burning.

The new tandetron accelerator of Atomki and the recently upgraded set of gamma-detectors provide improved conditions for studying radiative capture reactions. The topic of the PhD work will be the measurement of certain (p,γ) and (α, γ) reaction cross sections including all phases of the investigation from the design of the experiments to the final data analysis. The experiments will mostly be carried out at the tandetron and cyclotron accelerators of Atomki. In some cases, however, the work will be implemented in foreign institutions in the framework of international collaborations.

Supervisor: **Dr. Gábor Gyula Kiss**

PF2/456-17

Explosive nucleosynthesis scenarios

About 50% of the stable isotopes heavier than Iron are synthesized in explosive nucleosynthesis scenarios. In the so-called astrophysical *r* process – during the explosion of a type II supernova or a neutron-star merger – in series of rapid neutron capture reactions, exotic, neutron-rich species are created. After the neutron exposure, these isotopes are building up the heavy elements via consecutive beta decays. The so-called *rp* process takes place in x-ray bursts; via rapid proton capture reactions, isotopes located close to the proton drip line are formed. After the explosion, these isotopes decay towards the valley of stability, contributing to the abundance of the heavy proton-rich isotopes. In the modern radioactive isotope factories – e.g. RIKEN RIBF – the isotopes located on the path of these processes can be produced with high-enough rates and consequently their beta decay can be studied. These studies will lead to a better understanding of the *r* and *rp* nucleosynthesis scenarios. The PhD applicant will measure the half-life, the decay scheme and the delayed particle emission probabilities of some exotic isotopes using the recently developed detector systems.

The heavy, proton-rich (so-called *p* isotopes) are formed via the photodisintegration of the *s* and *r* seed nuclei. The so-called *γ* process takes place in the O/Ne layer of a core collapse supernovae. Due to theoretical and experimental reasons, instead of the (γ,p) or (γ,α) reactions, the inverse capture cross sections have to be measured. The accelerators and detectors available at Atomki are suitable to perform cross section measurements and elastic scattering experiments needed to understand the synthesis of *p* isotopes. The PhD student will carry out alpha- and proton-induced reaction cross section measurements – using the activation technique – and will derive the parameters of the alpha-nucleus optical model potential from the experimental alpha scattering angular distributions.

Supervisor: **Dr. Tamás Szücs**

PF2/457-20

Experimental study of solar and stellar nuclear reactions

In all stars including the Sun the released energy is produced via nuclear reactions. Additionally, those nuclear reactions are responsible for the building up the chemical elements in the universe. The Nuclear Astrophysics is an interdisciplinary field connecting the nuclear physics with astronomical observations and modelling, with the goal of understanding the chemical evolution of the universe and the solar and stellar behaviours. The experimental study of stellar and solar nuclear reactions is challenging due to the tiny reaction cross sections. It requires special efforts both in the planning and in the

implementation of the experiments. In a few cases, world wide unique equipment is also necessary. In many cases the detection of the tiny signals from the reactions is limited by the natural background radiation. To overcome this problem the shielding of the detectors, and the signal-to-noise ratio has to be improved with new ideas.

The main task of the PhD applicant will be cross section measurements relevant in the solar and stellar nucleosynthesis and energy production. All phase of the investigations, starting with the planning of the experiment, through the actual measurement and the final data analysis will be the duty of the student. The experiments will mostly be carried out at the accelerators of Atomki, but international collaborations are also foreseen. If the study needs, investigations can be carried out in foreign institutes, even in unique underground accelerator laboratories.

Supervisor: **Dr. Károly Tőkési**

PF1/458-18

Interaction of charged particles with atoms and surfaces

(See PF1/428-03),

Supervisor: **Dr. László Cséregi**

PF2/459-22

Study of astrophysically relevant nuclear reactions

The aim of the Nuclear Astrophysics is to understand the evolution and energy production of stellar objects, and to understand the production of chemical elements in the Universe. The solution of complex astrophysical models is required to gain insight in the different processes, in which the high precision study of astrophysically relevant nuclear reactions with their reaction rate is essential.

Thanks to the charged particle accelerators and the nuclear experimental apparatus (gamma-, neutron- and charged particle detectors, nuclear electronics, etc.) of the ATOMKI, the Nuclear Astrophysics Group of ATOMKI has decades-long experiences to study the relevant nuclear reaction on light and middle atomic number elements using in-beam gamma-spectroscopy and activation technique. The investigation of key reactions of hydrogen-burning and nuclear reactions of astrophysical r- and p-process belong to the main topics.

The main task of the PhD applicant will be the experimental study of nuclear reactions based on the investigation of nuclear products (light charged particles, electrons, gammas, neutrons etc.). The preparation and the planning of the experiments, performing the measurements (target preparation and characterisation, in-beam spectroscopy, activation technique) and the analysis of data will be in the focus of the candidate carried out mostly at the ATOMKI experimental apparatus.

Evaluation of novel techniques in radiotherapy

Radiotherapy, as the fundamental part of Oncology, has undergone a very fast technical development. Novel techniques result longer overall survival time among oncological patients, therefore maintain and support the quality of life is essential. The absorbed dose, the type of delivery and the quality of radiation are crucial to maximize the effectiveness and efficiency of radiotherapy, meanwhile reduce unwanted side-effects. Special dosimetric measurement and high impact quality assurance promote the security of radiotherapy. For a certain patient more radiotherapy plans have to be designed and the radiation oncologist can choose the best one for the case via continuous consultation with medical physicists.

Improvement in planning system and self-controlling methods may lead better quality therefore more radical radiotherapy, suggesting favourable clinical outcome.

Optimisation of the yield of laser generated neutrons

Acceleration of charged particles with lasers have been continuously investigated and developed over the past two decades, now reaching a level when user applications are becoming possible. The yield of laser-accelerated particles depends on the parameters of both the laser pulse and the target material. The neutrons generated via fusion reaction of accelerated ions are determined by the spectral yield of the ions as well as the nuclear interaction.

The aim of the present PhD thesis is to apply and / or develop a machine learning algorithm in order to maximize the yield of laser-generated neutrons of MeV energy range via D(d,n) fusion. The target-dependent optimisation is to be reached through varying the parameters of the laser pulse. The experimental campaigns of neutron generation are carried out at the ELI-ALPS Laser Research Infrastructure, while the related preparations are taking place in the laboratories of the University of Szeged and at ATOMKI, Debrecen.

III. Solid State Physics and Material Science program

Supervisor: **Dr. Zsolt Gulácsi**

PF3/42-93

Variational description of the strongly correlated systems

The systems intimately connected to the top questions of the present solid state physics (high T_c , heavy-fermions, quantum-Hall effect, system closely situated to the metal - insulator transition etc.) are strongly correlated. In these circumstances, the theoretical description (taken in extremely good approximations) of the models which reflect the essence of these systems (like the Hubbard model, extended Hubbard models, the periodic Anderson model, t-J model, etc.), represents one of the major problem of the actual theoretical solid state physics. The aim, connected to this subject, is to analyse, extend and develop the variational analysis of the mentioned systems and models.

Supervisor: **Dr. Sándor Mészáros**

PF3/43-93

Dynamics of magnetic flux in grain boundary junctions of high temperature

The structure of magnetic vortex lattice shows special character in HTSCs due to short coherence length. Grain boundary junctions play special role in determination of current transport, energy loss and magnetic properties. The problem is the description of magnetic vortices in the region where the superconducting order parameter is depressed. This depression gives rise to easy slip channels, where vortices can move. The task of the proposal is to study this phenomenon by observing its consequences in the electromagnetic properties of HTSC materials.

Supervisor: **Dr. Gábor Erdélyi**

PF3/45-93

Investigation of diffusion processes in oxide-ceramics

The mechanism of diffusion in ceramic oxides for example in alumina is not known. Tracer and chemical diffusion investigations may help to reveal the rather complicated defect structure of these materials and provide a better understanding of properties of metal-ceramic interfaces.

Supervisor: **Dr. Gábor Langer**

PF3/49-93

Production and investigation of physical properties of metallic multilayers

Production of metallic multilayers by magnetron-sputtering. Investigation of physical properties of one-dimensional nanostructures (electric, magnetic properties, interdiffusion).

Supervisor: **Dr. Zsolt Gulácsi**

PF3/413-95

Superconducting properties in layered compounds

The study of the superconducting properties in layered compounds is strongly connected to the continuously developing subject of high- T_c materials and artificial layered structures as well [1]. We want to focus in specially on specific properties connected to inter-layer effects like mediated inter-layer coupling [2] or inter-layer pair tunnelling [3]. We are interested to analyse the role of these effects in building up the superconducting properties of these materials, their influence on T_c and condensed phase characteristics, their relation to in-layer effects.

References:

- [1] Physica C235-240, Part 1-3/Dec. 1994, containing the contributing papers of High T_c conference, Grenoble, July 1994
- [2] Zs. Gulácsi, M. Gulácsi: Phys. Rev. B37. 2247(1988); Phys. Rev. B40, 708(1989); Phys. Rev. B42, 3981(1990).
- [3] W. C. Wu, A. Griffin: Phys. Rev. Lett. 74. 158 (1995)

Supervisor: **Dr. Dezső Beke**

PF3/414b-95

Production of nanocrystalline metastable alloys by mechanical alloying

Ball milling a very effective tool for the production of metastable nanocrystalline alloys. Production of different intermetallic compounds and extended solid solutions are planned to obtain materials of new interesting physical properties.

Supervisor: **Dr. Kálmán Vad**

PF3/415-95

Investigation of the magnetic flux dynamics in superconducting thin films

Traditional superconductors can be applied to two main purposes: to produce high magnetic fields and to develop superconducting instruments working on the basis of weak superconductivity. This classification can be used in the field of high- T_c superconductivity. In order to use high- T_c materials in magnet technology and superconducting electronics, we have to know the mechanism of current conduction, the parameters defining the critical current, the behaviour of the magnetic field inside superconductors, the mechanism of flux motions, etc. So, the investigation of macroscopic electromagnetic properties of high- T_c materials is important from the point of view applications. But it is also important from the point of view of basic research, because the mechanism of high- T_c superconductivity is still not known, furthermore, there are new phenomena in the magnetic flux structure due to the layered structure and short coherence length.

In the framework of the programme I intend to investigate the electromagnetic properties of superconducting thin films produced by the magnetron sputtering system installed jointly by Lajos Kossuth University of Debrecen and Nuclear Research Institute of

Debrecen in 1994. This includes performing measurements of magnetic and transport properties both in a DC magnetic field and in a high frequency electromagnetic field.

Supervisor: **Dr. László Kövér**

PF3/416-95

Chemical and solid-state effects in Auger transitions

(Same as PF1/420-95)

Supervisor: **Dr. Zsolt Gulácsi**

PF3/417-96

Exact solutions related to many-body systems

In the last period [1] a new method is developing that allows to deduce exact result related to $D > 1$ dimensional many-body systems, providing in this manner essential information connected to the system under study. As it is known up to this moment only $D = 1$ dimensional quantum systems were really accessible from exact solutions point of view. Because of this reason, the method under discussion seems to become extremely important in providing genuine information related to many-body models of higher dimensions. The application possibilities of the method are connected to main field of interest of the actual condensed matter theory, being related to the study of strongly correlated systems (high T_c superconductors, heavy-fermion systems, metal-insulator transitions, quantum-Hall effect), itinerant and localised systems as well.

The main idea of the new method is to deduce exact upper and lower bounds for the ground-state energy of the system based on approximation-free mathematical procedures, deducing in the same time the corresponding eigenfunction. Equating this two bound values, one can deduce in some parameter-space regions the exact ground-state of the system. The deduced results characterise those regions of the phase diagram that either were accessible up to this moment only by means of poor approximation procedures, or were completely out of a real theoretical control.

References:

1.) J. de Boer, S. Schadschneider, Phys. Rev. Lett. 75(1995)4298. A. Korepin et al., Phys. Rev. Lett. 74(1995)789.

Supervisor: **Dr. Dezső Beke**

PF3/421-97

Production and magnetic properties of nanocrystalline materials

Ball milling is a very effective tool for the production of metastable nanocrystalline alloys. Production of different intermetallic compounds and extended solid solutions are planned to obtain materials of new interesting physical properties.

Supervisor: **Dr. Gábor Erdélyi**

PF3/422-97

Grain boundary diffusion in nanostructured materials

In the last decade the research and development of nanostructured materials became an important and fast growing field of materials science. The peculiar properties of the developed materials can be attributed to the not negligible fraction of atoms being in the grain boundaries. The study of the grain boundary transport in such materials is of great importance in the point of view of applications.

We intend to investigate diffusion processes in nanostructured thin films prepared by magnetron sputtering by means of the so-called "first appearance technique". This involves monitoring of the diffusant at the back surface of the specimen and measuring the time necessary for the first appearance of the diffusant. Surface sensitive analytical techniques like AES, ESCA, (SIMS) can be used for such measurements. Traditional techniques can not be applied because the high temperature diffusion anneals, which would be necessary to get measurable profiles, would destroy the nanocrystalline structure of the specimen.

Supervisor: **Dr Zsolt Gulácsi**

PF3/423-97

Theoretical study of the periodic Anderson model

The periodic Anderson model, one of basic models incorporating main effects characterizing the strongly correlated systems, describes a hybridization type interconnection between a free particle band and a subsystem build up from electrons situated on periodically placed localized levels, Hubbard on-site interaction being present on every site. Based on the up to date knowledge, this model gives the best description of heavy-fermion many-body systems. Although this model concentrates main questions related to the actual solid state physics, its $d = 1$ dimensional exact solution is not known, and its $d > 1$ behaviour is almost completely open.

The theoretical study of the periodic Anderson model is in view of our group and we have important results related to its description (Zs. Gulácsi, R. Strack, D. Vollhardt: Phys.Rev. **B47** (1993) 8594.). Our aim is to enhance the scientific development in this direction taking into account the new results obtained in this field. The object of the proposed research is to deduce high quality, if possible approximation free results related to the periodic Anderson model in $d \geq 1$ dimensions in order to obtain main information connected to its physical behaviour. As a starting point we would like to use the method perfected by Strack and Vollhardt (Phys.Rev.Lett. **70** (1994) 2637.) that allows the calculation of an exact upper and lower bound for the ground state energy in a dimension independent fashion and superpose these two bound values within the parameter space. The development of the procedure is also in our attention.

Supervisor: **Dr. Zsolt Gulácsi**

PF3/424-97

Ordered phases in layered systems

The existence of layered systems give rise to a specific connection between two and three dimensional physical behaviour for many-body systems. Within a given plane the two

dimensional characteristics dominate with their strong restrictions related to the emergence of ordered phases. On the other hand, the layered system with its successively positioned layers interconnected via inter-layer interactions build up a three dimensional body whose characteristics are free from low-dimensional constraints regarding phase transitions, holding properties that reflect the signature of completely different physical parameters. At the border of these two system types one find extremely interesting physical properties, which are situated in the attention of the actual condensed matter physics being connected with main questions of large interest (the high critical temperature superconductivity belongs also to this category). Changing the coupling constants of inter-layer couplings we are able to push the model characteristics of layered system in the direction of both mentioned dimensional limits opening the perspectives for the study of the in-between region and to analyse properties emerging during one-plane to layered system parameter flow. We intend to study this subject concentrating not exclusively on superconductivity, but taking into account also other ordered phases as well like magnetic ordering, charge or spin density waves. The background for the proposed research on our side is present (see for example: M. Gulácsi, Zs. Gulácsi: Phys. Rev. **B42** (1990) 3981.; Zs. Gulácsi, M. Gulácsi, B. Jankó: Phys. Rev. **B47** (1993) 4168.). As a starting point, we would like to use a procedure based on Strack and Vollhardt (Phys. Rev. Lett. **70** (1994) 2637.) being interested also in the development of the method.

Supervisor: **Dr. Kálmán Vad**

PF3/425-97

Relaxation phenomena in magnetic structures

It is characteristic of magnetic structures in metastable states that their energy states decrease due to different relaxation processes. The relaxation can easily be investigated by measuring the magnetic momentum change in time. Especially the extremely fast and slow relaxation processes are interesting for us, which can be investigated by different methods. The validity of existing models can be checked by the structures on which we can perform our measurements, e.g. vortex structure in a superconductor or superparamagnetism in nanocrystal magnetic material. The candidate's task will be the investigation of the relaxation processes in these systems and compare the results to modern theories.

The experimental instruments and samples, e.g. different types of magnetometers, magnetic and superconducting materials are available for us. We intend to perform the measurements on magnetic materials in the framework of cooperation between the Institute of Nuclear Research and the Department of Solid State Physics of the L. Kossuth University.

Supervisor: **Dr. István Szabó**

PF3/427-98

Study of nanostructured materials by scanning probe microscopy

Experimental investigation of magnetic particles embedded in a non-magnetic matrix, magnetic multilayers, thin film structures and beaded thin films. Study of the film structure and magnetic domain structure by scanning probe microscopy. The primary aim is the investigation of the coupling between magnetic nanostructures embedded in a non-magnetic matrix.

Supervisor: **Dr. Dezső Beke**

PF3/428-99

Martensitic transformation in shape memory alloys

The martensitic transformation and the shape memory effect are among the most important topics of the modern physical metallurgy. The characteristic parameters of the transformation are strongly affected by the stress conditions as well as by the microstructure of the material. The dependence of the transformation properties on the above mentioned circumstances will be investigated by experimental methods in different (Ti-Ni, Cu-Zn-Al) shape memory materials.

Supervisor: **Dr. Gábor Erdélyi**

PF3/429-99

Grain boundary transport and segregation in intermetallic compounds

The study of grain boundary transport may contribute to a better understanding of the chemical interaction between impurities and boundaries and furthermore serves information on segregation processes.

In the framework of the project the investigation of Ni transport is planned in Ni₃Al, because this matrix has a great physical importance. Carrying out tracer measurements at rather low temperatures, to be in type C-kinetic regime, one can get direct information on the grain boundary diffusion coefficient and segregation.

Studying the pressure dependence of the transport, the elementary mechanism of grain boundary diffusion can be revealed, because the pressure dependence of the process, which can be characterized by the activation volume, may be significantly different for different diffusion mechanisms.

The necessary techniques, (tracer technique with high depth resolution, high pressure equipment, etc.) are available in our department.

Supervisor: **Dr. István Szabó**

PF3/430-99

Diffusion studies in intermetallic compounds

Intermetallics form an important group of modern materials. There are very scarce studies of the diffusion properties in these materials [1]. Beside the scientific interest (in problems like the strong correlated character of diffusion in ordered compounds [2]), the knowledge of diffusion data is needed for the understanding of high temperature creep processes.

The aim of the research is to characterize as completely as possible a selected alloy family using tracer diffusion and mutual diffusion measurements and/or with theoretical methods. We have a long tradition in the study of diffusion in metals by these technique [3,4,5]. Special equipments for the preparation (Ar arc melting), heat treatment (vacuum furnace), and characterisation (micro polisher, analytic microscopy TEM, SEM) are now also available.

[1] Landolt-Börnstein 22. (Ed. H. Mehrer): Diffusion in Solid Metals and Alloys.

[2] I. A. Szabó, M. Koiwa, S. Ishioka: Phil. Mag. **A63** (1991) 1137.

- [3] Defect and Diffusion Monograph Series No. 7. (1989) DIMETA-82 (Eds.: F. J. Kedves and D. L. Beke)
- [4] Defect and Diffusion Forum. Vol. 66-69 (1989) DIMETA-89 (Eds.: F. J. Kedves and D. L. Beke)
- [5] I. A. Szabó: Defect and Diffusion Forum. Vol. 143-147 (1997) 327.

Superrvisor: **Dr. Zsolt Gulácsi**

PF3/431-99

Theoretical study of $t - J$ model.

In the description of strongly correlated fermi systems the $t - J$ model plays an important role. The model is build up from itinerant fermions whose Hamiltonian besides the kinetic energy term contains a Heisenberg type interaction connecting particles situated on nearest neighbour sites. The starting Hamiltonian of the model can be deduced via an unitary transformation from the Hubbard Hamiltonian in the strong on-site interaction limit neglecting further terms with small coupling constants. This model is situated in the center of attention today because in the case of high temperature superconductors and heavy fermion systems a strong interparticle interaction based on spin fluctuations seems to be present, whose description presumably can be started from the $t - J$ model.

The $t - J$ model is extensively investigated in the scientific literature published in the last period. In spite of this fact, exact or accurate results related to it are known only in one dimensional case. Our aim is to extend the accurate description of this model to two and three spatial dimensions at least in some restricted domains of the phase diagram taking into account ground state and excited state characteristics as well. We are going to start the study based on the positive semidefinite operator decomposition used recently for the Hubbard model [1]. This procedure can be applied at least for the study of ground state properties in restricted areas of the parameter space. After this step the low-density limit will be analysed. In this case also excited state properties will be under study.

- [1] Zs. Gulácsi: Bull. Amer. Phys. Soc. **43**, 200, (1998).

Superrvisor: **Dr. Zsolt Gulácsi**

PF3/432-99

Theoretical study of lattice models in low-concentration limit

We are going to concentrate here on strongly correlated fermionic many body systems, especially the Hubbard model, in two spatial dimensions. We would like to start the study with small systems and to extend the deduced results for arbitrary large lattice. The aim is to analyse the hidden symmetry of the ground and excited states given by a small number of particles, if possible, in an exact fashion. From scientific point of view this is important for us because allows information collection regarding the development of exact solution procedures connected to two-dimensional quantummechanical many body fermionic systems. The deduced results will be used in the further study of the analysed systems. The subject is connected in the same time to the process of understanding of quantum-liquid properties given by 2D lattices in low density limit. This is important especially around the phase diagram domains where new condensed phases emerge in quasi-two-dimensional concrete systems (high T_c superconductors for example around their critical point).

The scientific background of the subject is substantial but poor. For example in the case of 2D Hubbard model, only the ground state wave-function explicit form is known [1], in spite of fact that the whole two-particle energy spectrum is available [2]. The problem presents a great interest [3] and is directly connected to the description of new condensed phases [4].

- [1] L. Chen, C. Mei: Phys. Rev. **B39**, 9006, (1989).
- [2] D. C. Mattis: Rev. Mod. Phys. **58**, 361, (1986).
- [3] O. Tjemberg: Jour. math. Phys. **39**, 6416, (1998).
- [4] A. C. Cosentini et al. Phys. Rev. **B58**, R14685 (1998)

Superrvisor: **Dr. Gábor Langer and Dr. Attila Csík**

PF3/433-99

Investigation of thermal stability of multilayers

Multilayers and superlattices are having considerable industrial interest because of their specific (magnetic, electronic, mechanical, optical etc.) properties. These properties are usually related to the high interphase and sometimes to the additional defects (grain boundaries, dislocations etc.). During annealing of multilayers their structure undergoes morphological changes, which usually destroy the favoured physical properties. Thus, investigation of the thermal stability and of the factors controlling structural changes of these multilayers is very important for the prediction of their lifetime.

Superrvisor: **Dr. Sándor Kökényesi**

PF3/436-02

Photostimulated processes in semiconductor nanostructures

Photostimulated structural transformations in light-sensitive chalcogenides and their influence on the optical, electrical parameters of amorphous layers will be investigated in layered nanostructures, where the composition, technology, thickness, interdiffusion of adjacent layers essentially influence the mechanism and value of transformations of above mentioned and other parameters. The results may determine the possibilities of applications for optical memory, fabrication of optoelectronic elements and the basis of fundamental and applied investigations of other types of amorphous semiconductor nanolayered structures.

Superrvisor: **Dr. Sándor Kökényesi**

PF3/437-02

Size-limited characteristics of semiconductor nanocomposites

The dependence of optical, electrophysical and other parameters of light-sensitive multicomponent chalcogenide-based semiconductor nanocrystals on the composition, dimensions of the crystallites and on the matrix composition, technology (semiconductor or dielectric glass, amorphous layer) as well, especially the effects of laser irradiation will be investigated and analysed as applicable for optical signal processing.

Supervisor: **Dr. Sándor Kökényesi**

PF3/438-02

Radiation stimulated transformations in amorphous material and its application in optoelectronics

The influence of electromagnetic radiation and accelerated particles (electrons, protons, neutrons and ions) on the structure, optical and mechanical parameters of amorphous wide-band semiconductor or dielectric materials, thin layers will be investigated in order to determine the mechanism of tailored transformations in these materials and their applicability for fabrication of optical elements, integrated optical structures.

Supervisor: **Dr. Ferenc Kun**

PF3/440-03

Study of non-equilibrium processes of magneto- and electrorheological fluids

Magnetorheological (MR) fluids are generally composed of micrometer sized magnetic particles of permanent magnetic dipole moment suspended in a non-magnetic viscous liquid. Electrorheological (ER) fluids have a similar composition but here the particles suspended in a passive liquid acquire an induced dipole moment in the presence of an external electric field.

In MR fluids, in the absence of an external magnetic field the particles aggregate due to the interplay of the dipole interaction and of the Brownian motion and build up complex structures like chains, rings, labyrinthin and compact objects. In the presence of an external field the particles form chains along the field direction which then organize themselves into regularly placed columns. Similar structure formation occurs also in ER fluids but solely in the presence of a driving field. Both MR and ER fluids are of great technological importance since the structures of particles formed change the rheological and optical properties of the colloid and makes possible to control these characteristics of the system by the driving field (smart fluids).

Rheological fluids allow also for the study of two dimensional colloidal crystals. It has been found recently that with dipolar particles placed on the surface of a viscous liquid two dimensional crystals can be formed with all the planar crystal symmetries.

In the framework of the present Ph.D. theme a theoretical study of the structure formation occurring in magneto – and electrorheological fluids has to be performed in a close collaboration with experimental groups of the field. The research covers the investigation of the aggregation kinetics, the cluster – cluster aggregation process, their influence on rheological properties of the colloids, furthermore, the study of the formation, stability and melting of two dimensional colloidal crystals is also included.

Supervisor: **Dr. Dezső Beke**

PF3/442-05

Investigation of semiconductor nanostructures

Supervisor: **Dr. Dezső Beke**

PF3/443-05

Nanodiffusion

Supervisor: **Dr. Ferenc Kun**

PF3/444-06

Study of fractures and fragmentation processes in solid states

Supervisor: **Dr. Dezső Beke and Dr. István Szabó**

PF3/445-07

Application of the magnetic noises in material science

Supervisor: **Dr. Gábor Erdélyi**

PF3/447-08

Diffusion phenomena in amorphous and crystalline systems

Diffusion and segregation phenomena will be studied in amorphous and crystalline semiconductors moreover, in industrial glasses. In semiconductors, the diffusion and segregation of some technically important impurities (Sb) are investigated. In MBE-grown, differently-stressed semiconductor structures our studies focus on the effect of mechanical stresses, moreover the effect of external pressure on diffusion and segregation phenomena. In industrial glasses, the diffusion of some impurities (Hg) will be investigated. The objective of the investigations is to find effective diffusion barriers in order to reduce the in-diffusion of mercury in glasses. This problem is closely related to the mercury consumption of energy-saving lamps. The diffusion experiments will be carried out in both systems by means of SNMS technique.

Supervisor: **Dr. Dezső Beke**

PF3/448-08

Smart materials: Investigation of metallic and polymer shape memory materials

The shape memory effect are among the most important topics of the modern physical metallurgy. The characteristic parameters of the transformations, leading to such behaviour, are strongly affected by the stress conditions as well as by the microstructure of the material. The dependence of the transformation properties on the above mentioned circumstances will be investigated by experimental methods in different metallic and polymer model shape memory materials. Effect of the nanocrystallinity and shape memory behaviour of different nanocomposite structures will also be investigated.

Supervisor: **Dr. István Szabó**

PF3/449-09

Supervisor: **Dr. Kálmán Vad**

PF3/450-09

Investigation of thin film solar cells

The development of Silicon based solar cells produced by vacuum technology is indispensable for increasing the efficiency and reducing the production costs. However, the increase of efficiency claims to perform a lot of research work and technological developments. Developing alternative solar cell structures (α -Si with higher efficiency, micromorf-Si or tandem α -Si/ μ -Si structures) claim to perform investigations with electron microscopes, to determine the constituents and their depth profile. We plan to perform this research project in close cooperation with the solar cell R+D program of the Research Institute for Technical Physics and Material Science. This scientific project is an experimental work: producing thin films (model solar cells) with the equipments operated in the two institutes, developing and using quality checking methods with secondary ion and neutral mass spectrometry, determination of constituents and their depth profile, measuring of the film thickness, measuring the parameters of films produced by other methods.

Supervisor: **Dr. Dezső Beke**

PF3/451-10

Investigation of diffusion and solid state reactions in thin layers: experiments and simulations

Investigation of diffusion and solid state reactions in nanocrystalline and amorphous layers by surface analytical techniques. Study of single interface movement by depth profiling technique. Computer simulation of phase growth kinetics, investigation of the role of stresses.

Supervisor: **Dr. Gulácsi Zsolt**

PF3/452-11

Characterization of strongly correlated systems

Strongly correlated systems are many-body quantum mechanical systems in which the inter-particle interactions are usually high, consequently the correlation effects are accentuated, hence low order approximations in the description are unsuitable. As a consequence, the theoretical understanding of these materials is based on high order, or non-approximated descriptions, and this state of facts provides the challenge in their study. Several systems of this type are known polarizing nowadays the scientific community: organic periodic systems, organic conductors, rare-earth alloys and compounds, layered systems, etc. The aim of the research topic is exactly the characterization of physical properties of these materials.

Supervisor: **Dr. Lajos Daróczy**

PF3/453-13

Statistical noises in martensitic materials

In martensitic materials different noise phenomena can be observed in the austenite and martensite phases as well as during phase transformation. Signals of different origin are characteristic for different physical processes. Correlations between different statistical noises can reveal important connections between the basic physical processes.

In all martensitic materials acoustic emission signals as well as noisy thermal signals (in case of sufficiently low heating rates) can be detected during the transformation. In

ferromagnetic shape memory alloys additional magnetic emission signals can be induced by temperature or deformation.

The detection and statistical evaluation of different signals are the most important aims of the proposed experimental work.

Supervisor: **Dr. Zoltán Erdélyi**

PF3/454-14

Study of nanostructured materials of high application potential

Materials scientists are facing industrial requirements to either construct materials with new properties or with same properties but lower cost of production. The current research topic is intended to face these requirements by creating nanostructured materials—primarily layered structures (e.g. nanolaminates, multilayers, core-shell structures)—of high application potential and studying their properties (such as thermal stability, electronic, optical). To reach this goal we will primarily use the experimental and theoretical (including computer simulation) tools and techniques available at our laboratory.

Supervisor: **Dr. Csaba Cserhádi**

PF3/455-16

Investigation of Kirkendall shift on the nanoscale

In a diffusion-controlled interaction, the movement of the Kirkendall markers during the interaction can be explained by the classical diffusion theory. The origin of this effect is the resultant vacancy flow, caused by the inequality of the intrinsic atomic fluxes in the lattice frame of reference, oriented towards the faster component, which is responsible partly for the development of stress free strain in the diffusion zone. The partial or full relaxation of the primary diffusional stresses can lead to the well-known Kirkendall shift. If the process is fast and complete then the stresses will be relaxed and the process is described by the well-known interdiffusion coefficient. In this case the Kirkendall shift is proportional to the square root of time. The effect is well described in binary systems in microscopic samples, but going down to the nanometer dimensions (thin films, multilayers, nanoshells or rods) additional problems arise. The characteristic distances between the vacancy sources/sinks can be comparable to the dimensions of the sample and a deviation is expected from the situation described above. In this case the diffusion is controlled by the slower component. We intend to study in this complex situation, the Kirkendall shift in thin films in different geometry (plane, cylindrical, spherical) in different metallic systems. The investigations have strong technological implications, since for instance the Kirkendall-plane is mechanically the weakest point of the diffusion bound.

The goal of this experimental project is to gain direct information from the composition profiles and the position of the marker plane on the nanoscale with a combination of experimental methods of SNMS depth profiling and synchrotron as well as neutron diffraction-based techniques, which are excellent methods to study processes on the nanoscale.

Supervisor: **Dr. Csaba Cserháti**

PF3/456-16

Atomic movements in 2 and 3 dimensional structures

We examine the movement of atoms on structures of planar and cylindrical geometry and of micro and nanometer size. We investigate the diffusion and solid state reaction process and its dependence on the radius of curvature.

This research is primarily experimental, from the planning and production of samples, through preparation, morphological and analytical investigations, to the final analysis of data. The diffusion couples will be examined and analyzed by microscopic methods. Models developed at our department can be used and extended to the tested systems in order to analyze the data.

Supervisor: **Dr. Dezső Beke**

PF3/456-17

Investigation of noisy character of phase transformations

It well known that martensitic transformations have a discontinuous, jerky character, i.e during it different (thermal, acoustic and – in ferromagnetic materials – magnetic) noises can be detected. There are also indications in the literature that diffusion and reaction controlled solid state reactions at low temperatures can have also a jerky character. Understanding the above phenomena have practical importance in improvement of materials in steel industry, shape memory alloys as well as in the nanotechnology of thin films and multilayers, where the requested property is produced by solid state reactions. Thus noises created by solid state phase transformations in the above materials will be experimentally investigated by differential scanning calorimeter (DSC) and by detecting acoustic and magnetic emission signals.

Supervisor: **Dr. Csaba Cserháti**

PF3/457-17

Risk based approaches in reliability assessment of corroded pressurised equipments in oil- and gas industry

Damage statistics of transit oil- gas pipelines and pressurised equipments in refinery industry. Overview of the corrosion damages in oil- and gas industry. Engineering methods of reliability assessment of corroded pipelines and pressurised equipments and their comparison. Basic principles of risk based inspection. Basic structure of API 581 procedures. Material databases of the corrosion resistance of materials applied in the refinery industry. Experimental verification of the corrosion resistance of the selected material(s) and the investigation of the corresponding parameter space. Metallurgical and chemical analysis of the specimens using light and electron microscopes (scanning and transmission), surface sensitive techniques (scanning neutral mass spectroscopy) as well as X-ray diffraction.

Research Activity: Damage statistics of transit oil- gas pipelines and pressurised equipments in refinery industry. Materials testing: Metallurgy and chemical analysis, studies by light and electron microscopes as well as X-ray diffraction.

Investigation of molecular-beam-epitaxially grown GaAs-based nano-structures

Till now, for the fabrication of the epitaxially grown III-V-based zero-dimensional nano-structures, the lattice-mismatch based strain induced technique was the only known method. Archetypal system of the clustered nano-structure is InAs on GaAs surface, where the strain-induced process leads to the formation of quantum dot. In this field, the droplet epitaxy serves as a new possibility. The droplet epitaxy is not only an alternative way to the conventional method but also a production method for number of zero-dimensional quantum structures such as ring-like, double-ring-like quantum structures or inverted quantum dots or quantum dot molecules. More information can be found under following link:

<http://www.intechopen.com/books/quantum-dots-theory-and-applications/quantum-dots-prepared-by-droplet-epitaxial-method>

Droplet-epitaxy is more flexible regarding the choice of the nano-structure material and also regarding the shape and distribution of the resulted quantum-structures. Furthermore, this technique is fully compatible with the technology of molecular-beam-epitaxy. For the control of the droplet-epitaxy, the knowledge of the growth kinetics is necessary, which is so far lacking the full theoretical understanding. The candidate is expected to join this research with the following contributions: evaluation of the measurements, calculations, modeling and simulations, experimental work with molecular-beam-epitaxy.

Required knowledges and skills: condensed matter physics, creativity, self-sufficiency, cooperation-ability, knowledge of English, practical sense (in the case of experimental works).

Study of nanometer scale surface atomic motion

Surface physics phenomena that take place at nanometer scale or atomic scale belong to the subject of modern physics. The research project is a surface physics project: study of surface and near surface atomic motions facilitated thermally, electrically or optically in films and film structures of a few nanometers thickness. However, at low temperatures (100-200C) the determination of activation energies which governs the atomic migrations and the determination of diffusion coefficients are not simple, and the experimental results are extremely insufficient. Moreover, atomic motions in thin films and in surface layers can significantly modify the physical parameters of a nanoscale system. Preparation of thin films and 2D layers is the part of the research program. We prepare different metallic and oxide layers by physical and chemical methods. The surfaces are studied by depth profile analyses with resolution of nanometer depth, by electron spectroscopy methods, as well as by scanning probe microscopy that is applicable to reveal the surface atomic motion and surface charge distribution. The student's tasks are learning these experimental techniques, taking part in the analyses and interpretation of data.

Modelling of parameters and sensitivity of plasmonic nanostructures based on metallic nanoparticles

The nano-sized materials have an essential role in the further development of material science. Besides of it, an important role has the studies of creation, investigation and possible application of nanostructured materials. Plasmonic nanoparticles, as one of the groups of nano-sized materials, has important properties, which make them possible materials for sensing application. Their size, shape, and material have an influence on the properties of these materials. The researchers are trying to optimize the parameters of creation to achieve the best sensing effectivity.

The aim of the work is to model, to study and to optimize the parameters of the created metallic nanoparticles and their sensitivity. The work is basically theoretically oriented, however, there is strong cooperation with experimental groups in this field. The work of the candidate consists of: get knowledge basic experimental and theoretical results in the field of the plasmon, plasmonic nanoparticles (possible creation technology and application), about the theoretical and experimental background of the localized surface plasmon resonance (LSPR) and surface-enhanced Raman scattering (SERS), will get skills in modelling of the parameters of the nanoparticles (material, size, shape) and their sensitivity. For this purpose, the candidate will investigate the influence of compositions, size, the shape of different metallic nanoparticles on LSPR and SERS sensitivity. Besides it, the optimal conditions of creation technology, application, and sensing of real chemical and biological materials will be studied as well. Besides it, the conditions and parameters of sensing of real chemical and biological materials will be studied as well. The results could lead to a new application of these materials in plasmonics.

Creation and investigation of plasmonic nanostructures based on metallic nanoparticles

The nano-sized materials have an essential role in the further development of material science. Besides of it, an important role has the studies of creation, investigation and possible application of nanostructured materials. Plasmonic nanoparticles, as one of the groups of nano-sized materials, has important properties, which make them possible materials for sensing application. Their size, shape, and material have an influence on the properties of these materials. The researchers are trying to optimize the parameters of creation to achieve the best sensing effectivity.

The aim of the work is to create and to study the parameters of the created metallic nanoparticles and their sensitivity. The work is basically experimentally oriented, however, there is strong cooperation with theoretical groups in this field. The work of the candidate consists of: get knowledge basic experimental and theoretical results in the field of the plasmon, plasmonic nanoparticles (possible creation technology and application), about the theoretical and experimental background of the localized surface plasmon resonance (LSPR) and surface-enhanced Raman scattering (SERS), will get skills in creation technology of nanostructures, in their investigation (focused on Raman spectroscopy and atomic force

microscopy). Further, the influence of the composition, creation technology, sizes and other parameters of metallic nanoparticles on its LSPR and SERS sensitivity and reproducibility will be studied. For this purpose, the candidate will create nanostructures with different technologies, investigate their parameters and sensitivity. During his/her work will get skills in creation technology of metallic nanoparticles (mostly in heat treatment and laser irradiation of thin metallic layers), and in their investigation (focused on Raman spectroscopy and atomic force microscopy). Besides it, the conditions and parameters of sensing of real chemical and biological materials will be studied as well. The results could lead to a new application of these materials in plasmonics.

Supervisor: **Dr. István Szabó**

PF3/462-19

Experimental study of nanomagnetic materials

Magnetic nanosystems: layer structures, nanoparticles and nanoparticle clusters can play an important role in future applications in both electronics and biomedical fields.

One such medical application is hyperthermia, which can target and kill cancer cells with the help of thermal energy generated by excitation of the magnetic nanoparticles with external magnetic field. During the theoretical research work in the institute, we have discovered a new excitation method that can increase the efficiency of heat production [1].

The aim of the research work is to test the theoretical results. In addition to the available magnetic measurement techniques, we have to create new measurement setups. A further task is the experimental testing of magnetic clusters and thin films with microscopy techniques. Another task is to perform simulation and calculations related to the experimental research.

[1] Iszály, Z., Lovász, K., Nagy, I., Márián, I., Rácz, J., Szabó, I., Tóth, L., Vas, N., Vékony, V., Nándori, I.: Efficiency of magnetic hyperthermia in the presence of rotating and static fields. *J. Magn. Magn. Mater.* 466 452-462, 2018.

Supervisor: **Dr. Viktor Takáts**

PF3/463-20

XPS-LEIS measurement techniques in surface science and materials science

X-ray photoelectron spectroscopy (XPS) and low energy ion scattering spectroscopy (LEIS) are among most prominent surface studying techniques for solid surfaces. While XPS gives both, quantitative and qualitative analysis from the samples topmost 6-8 nm width, LEIS gives information about topmost one atomic layer. XPS and LEIS measurement techniques requires UHV (Ultra High Vacuum) conditions, thus appropriate sample preparation technique must be learned. To analyze measured spectra mathematical procedures should be applied to achieve proper results for chemical state of the sample constituents. Research in this field assumes investigation of different type of samples. Among them are samples prepared in laboratory and industrial semiconductive materials or metal(alloy) samples as well.

Supervisor: **Dr. Viktor Takáts**

PF3/464-20

Ultra-high vacuum Scanning Probe Microscopy (UHV-SPM)

Investigation of atomically resolved surface relief or surface phenomena is possible by SPM (Scanning Probe Microscopy) operated under UHV (Ultra High Vacuum) conditions. The present research topic includes operation of STM (Scanning Tunneling Microscopy), AFM (Atomic Force Microscopy) and Kelvin-probe microscopy. For this purpose, knowledge of basic vacuum technique and sample preparation for UHV conditions are necessary. The main direction of the present scientific topic is the investigation of crystalline and polycrystalline surfaces properties and those electron structures. Also calibration of SPM on predetermined crystalline materials and special preparation of calibration samples are necessary to acquire. Thus achieved samples, prepared under UHV conditions, are appropriate for investigation of heat and laser light induced surface atomic motions.

Supervisor: **Dr. Gábor Katona**

PF3/465-17

Structural changes of thin films and heterostructures

Thin films and heterostructures often show unusual, peculiar properties. The understanding and exploiting of these properties requires knowledge on the connection between the structure and the properties, and also on the kinetics of possible structural transformations. In several cases to achieve the desired properties a multi-step process is required, e.g. annealing after deposition. The aim of the current research and the task of the candidate is to investigate structural changes and the kinetics of these in thin films and heterostructures and also to investigate the connection between structural changes and corresponding change in properties (e.g. magnetic, electrical, magnetoelectric).

Supervisor: **Dr. Károly Tókési**

PF3/466-20

Investigation of transport processes in simple and multilayer samples

There is a continuous interest and effort in the determination of optical constants of solids due to their importance in both fundamental research and applications. However, many materials still lack the data in the intermediate photon energy range around 20–50 eV. Furthermore, the available data in the current database usually consist of various energy regions measured by different groups and means; thereby the data may not be smoothly joined and inaccurate.

Task: to perform experimental and / or detailed Monte Carlo calculations on various (simple and multi-layer) samples to study the elastic (inelastic) backscattered electron spectra of electrons. Analysis of the spectrum distorting effect due to multiple electron scattering. Investigation of the surface effects. Review of the optical properties of solids based on the analysis of the “reverse” Monte Carlo method of energy loss spectroscopic spectra of backscattered electrons.

Requirements: Basic knowledge of atomic physics, quantum and classical physics.

Knowledge of programming language (Fortran, C, C++ etc).

Good skill of manuscript writing in English

IV. Physical Methods in Interdisciplinary Researches program

Supervisor: **Dr. Árpád Kiss**

PF4/412-94

Ion beam analytical methods in heritage science

Analytical techniques, especially physical methods considered as non-destructive, are more and more important in the complex research of cultural and natural heritage. With ion beam analytical techniques the concentration and distribution of elements can be determined in a given sample. The most widely used ion beam analytical techniques are PIXE (Particle Induced X-ray Emission), PIGE (Particle Induced γ -ray Emission, and RBS (Rutherford Backscattering Spectroscopy). For art and archaeological objects, minimising exposure while maximizing the obtained information is crucial. The optimum conditions for measuring sensitive materials must be determined through systematic investigations. It is very important to know about the unwanted effects of ionizing radiation and to avoid them as much as possible. Another aspect is how representative the obtained data are in relation with the entire object.

The aim of the proposed research is the thorough analysis of problems relating to the investigation of archaeological and museum objects and devising solutions.

Students interested in experimental work should apply.

Supervisor: **Dr. Mihály Molnár**

PF4/418-99

Environmental impact of nuclear power plants

The most important long-lived radioactive gases discharged during nuclear power plant operation are ^3H , ^{14}C and ^{85}Kr . Tritium is emitted into the environment in the form of HTO and HT, while radiocarbon is discharged as hydrocarbon and carbon dioxide. Stack samplers were developed and continuously operated to obtain integrated samples for measurement of tritium and radiocarbon of all chemical species as well as for ^{85}Kr . Sample preparation and enrichment methods were developed. Low-level gas proportional counting system and liquid scintillation counters are used for activity measurements. The normalised releases of the global contaminants were determined. Radiocarbon and tritium are monitored in the environmental air and local groundwater. Radionuclide transport calculations of tritium in the Paks aquifer were carried out and contamination maps were created.

In the framework of the research topic it is necessary to interpret the existing environmental radiocarbon and tritium results, make calculations in connection with tritium and radiocarbon transport in the atmosphere and hydrosphere, carry out sampling campaign of the observation wells around the nuclear power plant and measure the ^{14}C and tritium activity concentrations in the environment. ^{85}Kr should be measured in the stacks.

Radon in mofettes

The final product of post-volcanic activity is the carbon dioxide gas, which is called dry mofette. Examples of mofettes are the Torjai-Büdös-cave in Transylvania, Romania or the carbon dioxide seepage in Mátraderecske, Hungary. Along its pathway to the surface the deep origin gas also intakes different radon isotopes from the rocks and soils. Therefore the variation of surface radon exhalation can be a tracer of spots of carbon dioxide outgassing, which occurs most at near surface faults. On the other hand, mofettes are often used for therapeutic treatments in the form of dry carbon dioxide spas, where the risks, associated with radon exposures should also be a concern. The aim of this work is the study of spatial and temporal variation of radon isotopes in mofettes and in dry carbon dioxide spas and the analyses of the results in environmental physical, geochemical and environmental radiation protection points of view.

Improvement of solid state nuclear track-etched detector techniques and their applications.

The first observation of tracks (radiation damage) in mica from the ^{235}U fission fragments was made by Silk and Barnes in 1959 with a transmission electron microscope (TEM). After this observation within a few years extensive investigations were carried out for the enlargement of tracks produced by different charged particles using the chemical etching process. This method rendered the magnification of etched tracks to sizes where they could be viewed with an ordinary optical microscope possible. The dimension of the damage region was enlarged with about four orders of magnitude by the etching techniques i.e. up to $\sim 10\mu\text{m}$ both in crystal and polymer materials. In the crystal the damage consists of vacant lattice sites and of interstitial ions or atoms while in the polymer new chain ends and other chemically reactive sites are formed. A number of scientific and practical applications were based on the thin polymer foils of large dimensions (nuclear science and engineering, particle physics, cosmic ray astrophysics, geology, archaeology, sub-oceanic geophysics, space research, meteorite and lunar studies, dosimetry, etc.). The wide range of applications required the development of reliable and reproducible evaluation methods especially for the determination of indoor and outdoor concentrations of radon (^{222}Rn) needed for the estimation of the dose caused by the natural background radiation.

The main aim of this investigation is to respond the question whether is there a definite correlation between the number of tracks measured by a given detector (e.g. CR39) and the deposited dose value. These investigations require the determinations of those external parameters which can influence the number of Rn atoms and their decay products reached the surface of the detectors and the detection efficiency of the tracks produced by these radioactive atoms. The latter require further investigations on the mechanism of formation of tracks, on the effect of thoron (^{220}Rn) and on the techniques of track-etching and counting. The results of such investigations can contribute significantly to the extension of the applications of the Solid State Track-etched Nuclear Detectors.

Investigation of the behaviour of radon and its progeny in outdoor and indoor air

A sensitive grab sampling method for the determination of radon (^{222}Rn and ^{220}Rn) progeny in air has been developed in the previous years and its characteristics were investigated. The hardware and the software for this method will be developed further and the investigation of its characteristics continues within the scope of this research topic.

The measurement of the radon concentration by active monitoring and the continuous measurement and registration of the weather variables make it possible to investigate the dynamics of radon and progeny outdoors and indoors (flats and caves) in the function of the environmental circumstances. From the results, useful conclusions can be drawn about the exposure to men from radon at different places.

Noble gases dissolved in fluid inclusions of dripstones as climate change indicators

The Earth's climate is always changing, so does the climate of our days. While the climate of the past was changing due to natural processes, the climate change of today is attributed to human impact. The knowledge on what happens in the future is scarce, unless good climate models are developed that are inspired to give prediction to this question. To verify recent climate models, they have to be able describe changes in the past. Thus, the more known the past climate, the more precise the predictions can be made. The investigation of past climate change is always based on geological archives, such as ice cores, marine or lacustrine sediments, speleothems, groundwater etc. Several different characteristics can provide useful information with regards to the climate, for instance trace elements, isotopic composition, pollen composition, thickness of the different layers.

One of the most frequently applied archive is groundwater. The measurement of dissolved noble gases in groundwater as temperature indicators has become an established method to reconstruct glacial/interglacial temperature changes. The noble gas palaeothermometer is generally regarded as a precise indicator of absolute temperature, which constitutes the importance of this method compared to other palaeoclimate proxies in particular for calibration of climate models.

However, groundwater as a palaeoclimate archive has several limitations. A more promising archive could be fluid inclusions in speleothem and other carbonate deposits from caves. In principle it is possible to determine noble gas concentrations in such trapped water.

The aim of the PhD work is to develop a precise method for determination of noble gas temperatures on fluid inclusions of stalagmites and stalactites. The work includes measurements of noble gas concentrations in very small water samples, production of artificial dripstones in controlled laboratory circumstances, test of the reliability of the temperatures calculated from noble gas concentrations, then investigation of old dripstones of known ages and calculation of temperature changes in the past.

Ion beam microanalysis in geological research

Geological samples are — in general — complex aggregations of crystalline and amorphous components. By their investigations conclusions can be drawn for the geochemical processes taking place in the earth's interior as well as for impacts on the earth crust. Study of their chemical composition plays a key role in the exploration of deposits of raw materials and processing of minerals.

Ion beam analytical methods based on a few MeV accelerator facilities (Particle Induced Gamma-/X-ray Emission Analysis: PIGE/PIXE, Rutherford Backscattering Spectrometry: RBS, Nuclear Reaction Analysis: NRA) are widely used in geological research due to their non-destructive nature, excellent sensitivity, lateral and depth resolution, and the ability for standardless analysis. The combined use of Scanning Nuclear Microprobes and ion beam methods allows the determination of elemental composition down to microscopic sizes by $1 \times 1 \text{ } \mu\text{m}^2$ lateral and — depending on element and sample — 10-20 nm depth resolution and detection limits between 1-100 ppm.

In cooperation with the Department of Mineralogy and Geology of the University of Debrecen comparative geochemical investigation of obsidian samples from various sources were carried out by ion beam methods, minerals and rocks were investigated. Significant efforts were made in the field of analysis of cosmic microobjects (micrometeorites, spherules) as well as impact materials made during meteoritic impacts (e.g. Barringer Meteorite Crater, Arizona).

This research inspires the continuous development of ion beam analytical methods with respect to sensitivity, detectable elements, accuracy, lateral distribution and detection limits. Therefore, we aim to study the underlying physical backgrounds of 2D quantitative micro-analytical methods (especially micro-PIXE technique), moreover, the accurate experimental determination of a part of the fundamental parameters used in data bases.

Supervisor: **Dr. István Csige**

PF4/430-09

Characterization of radon potential of building sites

The largest part of the exposure of the public from natural background radiation comes from the inhalation of the daughter products of radon gas at homes. This exposure plays an important role in the induction of lung cancer. In most of the cases, when high indoor radon concentration occurs at homes, the responsible source is the soil. Effective protection against radon at home requires – among other things – to determine the radon source potential of building sites before a new building is raised on it. The aim of this work is to improve the methods developed to characterize the radon potential of building sites.

Supervisor: **Dr. Mihály Molnár**

PF4/431-09

Development of alternative methods for detection of fossil carbon-dioxide in the atmosphere

Aim of the work is to develop simpler and less expensive methods for the estimation of atmospheric fossil CO₂ contribution. Till now only a few observation stations (<10) can fulfil the requirements of direct measurement of this parameter which is limited by the Kyoto protocol. In the framework of the PhD work a multipurpose long-term integrated sampling

technique should be developed to collect only a single whole air sample for direct measurement of fossil CO₂. The candidate has to investigate the possibility to apply carbon-monoxide (CO) as a quantitative proxy for fossil fuel CO₂ in the atmosphere in this region using a high precision on-line monitoring system, developed in this work. The representativeness of tree ring ¹⁴C record for atmospheric signal has to be also tested in several different localities in Hungary and Czech Republic. Using tree ring radiocarbon AMS measurements (prepared in Hungary and measured in Italy) in special localities (K-Pusztta and Hegyhátsál in Hungary) where continuous observations of CO₂ mixing ratio was made in the past it will be possible to reconstruct the atmospheric fossil fuel CO₂ contribution in the last three decades.

Supervisor: **Dr. István Rajta**

PF4/432-09

Proton Beam Micromachining

Technologies for the fabrication of microcomponents, microsensors, micromachines and micro-electromechanical systems are being rapidly developed, and represent a major research effort worldwide. There are a few patterning technologies currently being utilized in microstructure production (e.g. optical lithography, electron beam lithography, focused low energy ion beam machining, etc.). These techniques are essentially restricted to the manufacture of thin microstructures, since optical, electron and low energy ion probes have limited penetration depths typically only a few micrometers in resist materials. While the production of thin microcomponents is proving very successful (e.g. in the manufacture of accelerometers, gyroscopes, etc.), there is a growing need for techniques that are able to produce true 3D microstructures (e.g. for the production of microchannels, fluid flow sensors, valves, microcavities, etc.).

High Aspect Ratio Micromaching (HARM) technologies allow the fabrication of thick 3D structures usually using an ionising probe which is capable of penetrating deep into the resist. LIGA (Lithographie Galvanoformung Abformung), which utilises X-rays; and MeV energy protons (PBW - Proton Beam Writing) represent two such techniques, and with these probes penetration depths of ~100 µm are possible. Using HARM technologies several microstructures (such as molds, gears, channels, etc.) have been fabricated.

In the LIGA process, intense X-ray radiation from a synchrotron is passed through a specially prepared mask and the transmitted X-rays are used to expose a pattern in a suitable resist material. PBW differs from LIGA in that the technique is a direct write process, and thus offers the advantage that the process does not require a mask. Hence, PBW is ideal for basic research of the resist materials, and for prototype manufacturing of microstructures. Presently a project proposal is under evaluation at NKTH aiming PBW production of LIGA masks.

The supervisor has been working in Singapore and took part in the developing of the PBM method, and has established the technology available in Debrecen, Hungary at his home institute.

Radiation damage and radiation protection problems caused by fast neutrons

Mixed fields of radiation environments with fast neutron components are present

- at nuclear energetics systems: fission and fusion reactors, systems for transmutation of nuclear wastes,
- at high intensity fast neutron sources used for material science purposes: SNS, J-PARC, ESS, IFMIF, etc.,
- at particle accelerators and at experiments of high energy physics (HEP),
- in space research,
- in avionics,
- in military applications,
- in radiation therapy.

Neutrons interacting with atomic nuclei of media exposed to a radiation environment with neutron component can induce a) atomic displacement cascades leading to radiation damage and b) nuclear reactions that can lead to formation of radioisotopes and, thus, induced radioactivity of the irradiated media.

The aim of the planned research is modelling radiation damage and radiation protection problems via computer simulations and experimental methods. Problems important from the point of view of the European Spallation Source (ESS) will be addressed, too.

Detection and identification of illicit drugs, explosives and anti-personnel landmines using neutron based techniques

The main elements (H, C, N, O) of these materials can be observed by the elastic and inelastic scattering of neutrons. For the detection of anti-personnel landmines (APMs) hand-held neutron detector is available in the Institute of Experimental Physics in addition to the metal sensor. These detectors can be used for field applications by fast scanning of the soil surface and observation of APMs by the anomalies in the reflected neutrons. The reflection of thermal and/or epithermal neutrons rendered to the radioscopy of bags on conveyor belt possible. These methods need further improvements on their sensitivity and reliability. For the detection of carbon and oxygen the 4.44 and 6.13 MeV gamma lines can be used produced by inelastic scattering of fast neutrons, e.g. $E_n > 10\text{MeV}$ produced in D-T reaction. For the detection of C, N and O elements and their atomic ratios the measurements of spectra of backscattered neutrons by a neutron spectrometer based on an NE213 scintillation detector. It is required the comparison of experimental data by the results of model calculations, e.g. by the MCNP code.

Supervisor: **Dr. Julius Csikai and Dr. András Fenyvesi**

PF4/435-10

Investigations on excitation functions of neutron induced reactions in the 8-12 MeV problem range

A comprehensive review published by the IAEA-NDS in „Reference neutron activation library”, (IAEA-TECDOC-1285, VIENNA, 2002) has shown that the excitation functions are scanty and discrepant especially in the 8-12 MeV incident neutron energy range. Very few data are available for the production of short-lived isotopes. These data could be investigated by using the fast pneumatic sample transfer system developed at the MGC-20 cyclotron of ATOMKI in the last years. The running time is about 10 second between the irradiation and measuring sites. The excitation functions are required to measure by activation method for (n,n'), (n,p), (n,d) and (n, α) reactions. The multiple-foil method has been developed for the determination of spectra of incident neutrons. Data should be compared with the model calculations.

Supervisor: **Dr. Ferenc Kun**

PF4/436-11

Study of fractures and fragmentation processes in solid states

Supervisor: **Dr. Ferenc Kun**

PF4/437-11

Dynamics and statistics of avalanches in complex systems

Driven dissipative systems composed of a large number of interacting elements have the generic feature that as a consequence of external driving a metastable state emerges from which the system escapes by a relaxation mechanism. The process of driving is typically slow, however, the relaxation occurs on a much shorter time scale leading also to the restructuring of the system on the microscopic level in avalanches. These dynamical features are characteristic for Earth crust and for heterogeneous materials subject to a loading process, where driving is carried out by the slowly varying external load, and the relaxation mechanism is provided by avalanches of earthquakes and micro-fractures.

The goal of the research project is to investigate the dynamics and statistical features of avalanches which emerge in complex systems. Based on the analogy of earthquake and of the creep rupture of heterogeneous materials we are going to work out a generic model, which is able to reproduce the universal features of the probability distributions of quantities describing avalanches. Our main goal is to clarify under which circumstances one can predict the imminent catastrophic event of rupture or earthquakes based on the dynamics of avalanches. The research is mainly of theoretical nature, it requires analytical calculations and computer simulations using Monte Carlo and molecular dynamics techniques. The project is carried out in a close cooperation with experimental partners so that the evaluation of experimental results is also part of the research tasks.

Supervisor: **Dr. Zsófia Kertész**

PF4/438-11

Characterization of atmospheric aerosols by nuclear microanalytics

Atmospheric aerosol concentration is one of the most important characteristic of air quality. Due to their negative impact on human health and their influence on climate forcing and global warming quantitative characterization of airborne particles is becoming increasingly important to governments, regulators and researchers

The aim of the PhD work is to characterize the atmospheric aerosols and to study the human exposure due to particulate matter. The proposed work fits into the aerosol research done in the Laboratory of Ion Beam Applications in the ATOMKI. The task of the PhD student is to join this research, and take part in the development of sampling, sample preparation and analytical methods, and the complex characterization of airborne particulate matter.

Supervisor: **Dr. István Nándori**

PF4/439-12

Theoretical study of relaxation in magnetic nanoparticle systems

The study of relaxation of magnetic nanoparticle systems or more general the mechanism of magnetization reversal in single-domain ferromagnetic particles has a great relevance. Besides ferromagnetic resonance the dynamics of the magnetic moment of nanometre-sized single-domain particles is of interest in connection with a number of applications. For example, at low frequencies of the applied field, in cancer therapy by hyperthermia the specific loss power should be maximized. At larger frequencies, in case of MRI devices just the opposite requirement prevails: losses must be minimized. Therefore, due to the various numbers of possible applications, up to now the study of relaxation mechanisms of magnetic nanoparticles is a very active research field. The dissipation in case of the linearly polarized applied field has been analyzed in great detail, however less is known on the circularly polarized one.

The long-term goal of the present research plan is to consider the relaxation of magnetic nanoparticle systems under circularly polarized applied field. Theoretical study has already done for the isotropic, single-particle case. The next step is to generalize the previously obtained results to the anisotropic case and to develop and apply a statistical description of magnetic nanoparticle systems needed for the comparison to experimental data.

Supervisor: **Dr. István Csige**

PF4/440-13

Hydrodynamic modeling of contaminated subsurface flows

In recent years, increasing attention was paid towards the contamination of groundwater with hazardous (including radioactive) industrial wastes. These studies rely heavily on model calculations that describe the transport of pollutants. The purpose of this research topic is to develop such geological-physical, mathematical, numerical and computer models and to apply them in case of radioactive waste disposal facilities in Hungary. To do this research finite difference (Visual Modflow) and finite element (COMSOL Multiphysics, Subsurface Flow Module) computer applications are available.

Supervisor: **Dr. László Palcsu**

PF4/441-14

Development and application of novel analytical methods in palaeoclimatology and

isotope hydrology

Our research is based on state-of-the-art analytical methods which have been established in our laboratory in the last two decades. These methods have to be further developed, on the other hand, new research approaches have to be worked out in the field of isotope hydrology and palaeoclimato science.

Our plans include the following topics:

- dating of very fresh water in karstic springs using the cosmogenic ^{35}S isotope.
- studying palaeoclimate oscillation using the oxygen isotope composition of alpha-cellulose extracted from peat species (*Sphagnum*) collected in peat bogs.
- dating of speleothems with the $^{230}\text{Th}/^{234}\text{U}$ method.
- reconstruction of past cave environment with the measurement of hydrogen and oxygen isotope ratios of water inclusions of speleothems.
- reconstruction of palaeotemperatures in caves by means of noble gas solubility temperatures of fluid inclusions of speleothems.
- palaeoclimate reconstruction based on groundwater dating and noble gas temperatures.

Supervisor: **Dr. Róbert Erdélyi**

PF4/442-15

Role of macrospicules in the dynamics of the solar atmosphere

The high, few million degrees of K temperature of solar atmosphere is one of the unsolved mysteries of modern astrophysics that is also at the focus of a number of major international research institutions and funding agencies (ESA, NASA, JAXA, etc...). This proposal is along this line, and focuses on to examine the dynamics of the solar atmosphere in terms of macrospicule.

Macrospicule are jet-like elongated magnetic plasma structures in the solar chromosphere transporting energy and momentum, with a few 100 km/s propagation speed, into upper atmosphere of the Sun. Their typical lifetime is around 15-25 minutes, their length could be up to 80 Mm while their radius is relative small (1-2 Mm) when compared to their length. Macrospicule can be distinguished by their spatial properties and often are seen as one of two types:. They could develop in open coronal holes or in the Quiet Sun where the properties of the magnetic fields have a closed structure.

During this project, by using the Atmospheric Imaging Assembly (AIA) instrument on-board the SDO (Solar Dynamics Observatory) satellite -of which the Supervisor is an Invited Advisor by NASA-, we will determine the key physical properties of macrospicules in great details. One of the crucial point of our proposal is to establish and determine the temporal behaviour of the occurrence of macrospicule and to examine their relationship with the Solar Cycle. We have already found that the temporal variation of length of macrospicule shows around a 2-year fluctuation. This finding could be paradigm-changing as this may put a serious constrain on the solar dynamo theory. Our next step is to continue this study based on a larger dataset and derive statistics. Furthermore, all of the provided wavelengths of the AIA instrument will be used in the future, to repeat the above studies, allowing as to gain a 3D insight (i.e. also as function of height) into the relation between macrospicules and solar atmospheric dynamics.

To estimate the non-thermal energy transport of these jets from the lower solar atmosphere into the solar corona and solar wind, will be a crucial step in order to understand

the coronal heating process(es). The rotation velocity profile of macrospicule could be a key parameter here to reveal the properties of this energy transport. The recently launched Interface Region Imaging Spectrograph (IRIS) satellite may provide us the required observations about the rotation velocity profile, what we will study and compare to SDO data.

The Transition Region is a thin, elastic membrane-like region of the solar atmosphere in terms of MHD wave theory. Macrospicules, during their rise, hit this region and generate horizontal rippl-type of MHD waves called Transition Region Quakes (TRQs) that may play dominant roles in the heating the lower solar atmosphere. We will focus on investigating the relation between macrospicules and TRQs in order to reveal what their relevance is in plasma heating.

The last phase of the project will be to investigate the relation (if any) between macrospicules and solar dynamo operating at the convection zone. Here, we plan to carry out complex numerical simulations using SAC (Sheffield Advanced Code) and will collaborate with colleagues from DHO (Debrecen Heliophysical Observatory).

Last but not least, an important part of the project will be the use of the instrument suite available at DHO, in particular to further the Debrecen Sunspot Catalogue, that may hold key information for investigating the origin of solar macrospicules.

Supervisor: **Dr. Tünde Baranyi**

PF4/443-17

Study of solar activity and solar irradiance

The amount of the solar energy output carried by the electromagnetic radiation is one of the basic data of the Sun. It is one of the longest and most fundamental of all climate data records derived from space-based observations. Variations in the spectrum of solar irradiance (the Solar Spectral Irradiance, SSI) or in the total (spectrally integrated) solar irradiance (TSI) may affect a number of radiative, dynamical, and chemical processes in the Earth's atmosphere, and the climate. The space-borne measurements found a TSI variation of ~0.1-0.3%, while the range of SSI variation depends on the wavelength of light. The TSI and SSI exhibit variations on various time scales caused by magnetic features in the solar atmosphere. Considerable international efforts are devoted to track the irradiance variations and to clarify the roles of the solar magnetic features in them. At present, there are no physical models available but proxy-based models and semi-empirical models have been developed to model the measured data and to extend the studies to wavelengths where no direct irradiance measurements exist and backwards to the times before the start of the irradiance datasets. The performance of proxy models that are based on daily indices representing the darkening of sunspots and the brightening by faculae and small magnetic elements strongly depends on the precision of the proxies. The Debrecen sunspot databases are widely acknowledged as the most precise and detailed empirical bases of the sunspot activity and the datasets of photospheric faculae are unique. One of the research tasks of the candidate is to improve the input proxies and to check the impact on the output. The other planned task of the candidate is to find answers to some open questions of irradiance modeling on contributions of various solar features by using statistical methods and creating proxy models. For example, the supervisor's previous results show that the darkening effect of a sunspot group may not only depend on the area and contrast of spots but it may also depend on the evolutionary phase and morphology of the group. Among other things, it will be the candidate's task to verify or falsify these results by using the new high-accuracy irradiance observations e.g. provided by

the Total and Spectral Solar Irradiance Sensor (TSIS) mission after its launch expected in October 2017.

Supervisor: **Dr. Róbert Erdélyi**

PF4/444-18

Magnetohydrodynamic waves in the solar atmosphere

High-resolution ground- and space-based magneto-hydrodynamic (MHD) waves are ubiquitously observed in the solar atmosphere. They are very important as they may have dominant contribution to the plasma heating present in the solar atmosphere, that is one of the key puzzles of modern astrophysics. Another key aspect of solar atmospheric MHD wave research is that these waves may be used to diagnose the magnetised solar plasma where they propagate. This project is to further the currently available MHD wave theory in inhomogeneous waveguides. The theory will be applied to a number of solar structures from pores, magnetic bright points to solar jets, called spicules.

The study will involve mathematical modelling complemented with observational data analysis using high spatial, temporal and spectral resolution solar telescopes. The developed MHD wave theory will be justified by validating the obtained analytical results with observational data.

This project requires excellent skills in mathematical modelling complemented with interest in taking observations by either ground- or space-based telescope. Further, the project also likely requires collaboration with colleagues from Solar Physics and Space Plasma Research Centre (SP2RC), University of Sheffield (UK). Therefore, it is anticipated the student to spend some time at SP2RC within the framework of Erasmus+ or otherwise.

Supervisor: **Dr. Róbert Erdélyi**

PF4/445-18

Developing state-of-the-art Space Weather forecast tools

The production of flares and Coronal Mass Ejections (CMEs) from solar active regions (ARs) is still not well understood in spite of their huge importance to Sun-Earth connections, in particular, to protect mankind and our sophisticated technological systems that might be at considerable risk from high-speed charged particles blowing often abruptly off the Sun. These most energetic eruptions of the entire Solar System follow the 11-year solar cycle. At the peak of the cycle, several dangerously high-intensity class flares and CMEs may occur (i.e. around monthly 2-3). Most solar flares and CMEs originate from magnetically active regions around sunspot groups. To make a leap forward in Space Weather prediction, the student will generalise our forecast method, by applying it to the Interface Region and low corona in 3D, in order to identify the optimum height for flare/CME lift-off prediction in the solar atmosphere. Here, we expect to considerably increase the current forecast capability, with having important practical implications in our high-tech-driven world. In particular, the student will aim (i) to investigate the pre-flare/CME dynamics and the related physical processes in the 3D solar atmosphere by constructing the magnetic topology above ARs, and (ii) to track their temporal evolution by applying WGM. These aims will be realized by the objectives of (i) acquiring knowledge to implement potential and non-linear field exploration techniques; (ii) create a data catalogue of 3D magnetic mapping of AR(s). The student will also (iii) employ the next-generation high spatial- and temporal-resolution sunspot data,

provided by a combination of ground- and space-based magnetogram, white light and EUV observations, in particular with the complementary use of the solar observations of the novel Gyula Solar Telescope.

This project requires interest in taking observations by either ground- or space-based telescope. Therefore it is expected that the student may undertake such work with ground-based solar observatories. Further, the project also likely requires collaboration with colleagues from Solar Physics and Space Plasma Research Centre (SP2RC), University of Sheffield (UK). Therefore it is anticipated the student to spend some time at SP2RC within the framework of Erasmus+ or otherwise.

Supervisor: **Dr. Róbert Erdélyi**

PF4/446-18

Studying the evolution of solar faculae over the solar cycle

The generation of solar faculae and the evolution of their properties during the 11-year solar cycle are still not well-understood in spite of their importance to Sun-Earth connections. In particular, this has relevance in the context of space weather research in order to develop efficient forecasting to protect mankind and our sophisticated modern, GPS-based technological systems that might be at considerable risk from the Sun caused by solar storms. The relation between solar faculae and the solar cycle is a very exciting and new area of research. There are considerable potentials that a better understanding of such a connection may shed light on the yet unclear details existing between the evolution of solar global magnetic fields governing space weather and the related space weather forecasting.

Most solar faculae originate from magnetically active regions around sunspot groups. However, the loci of origin of facula do migrate from the equator towards the poles during the solar cycle. There is mounting evidence that there are both temporal and spatial correlations between the various migration paths of these loci. These correlation patterns need to be fully investigated, understood and modelled.

To make a leap forward, the main aim of this research by the student will be to statistically map, interpret and model these migration coherences. These aims will be realised by the specific goals of i) building up a database and investigating the dynamics of facular migration on the surface of the Sun; and ii) analysing and modeling the temporal evolution of facular migration.

The student will have the specific tasks of (i) acquiring and familiarising with the literature necessary, in particular, the long-term evolution of solar global magnetic field (i.e., dynamo theory and the new theory of double dynamo); (ii) delivering a solar facular catalogue for the period of a solar cycle; (iii) employing the next-generation spatial- and temporal-resolution facular data, provided by a combination of ground- and space-based magnetogram and white light observations. The latter will be aided by the complementary use of observations provided by the Solar Activity Magnetic Monitor (SAMB) of the novel Gyula Bay Zoltan Solar Observatory (GSO); and (iv) analysing, interpreting and modelling the obtained data in terms of the solar double-dynamo theory.

This project requires interest in taking observations by either ground- or space-based telescopes. Therefore, it is expected that the student may undertake such work with ground-based solar observatories. Further, the project also requires collaboration with colleagues from the Solar Physics and Space Plasma Research Centre (SP2RC), University of Sheffield (UK). Therefore, it is anticipated from the student to spend some time at SP2RC within the framework of Erasmus+ or otherwise.

Development and application of isotope analytical methods to identify natural and antropogenic carbon sources

Within this research, the candidate will develop procedures for sampling, sample preparation and measurement of the most modern stable isotope and radiocarbon analytical methods in order to identify different natural and antropogenic carbon sources and the presence of these sources in media. The main targets of the investigations planned: groundwater and aquiferic water, air and aerosol, plants from various contaminated sites, certain industrial products and wastes. Within these, separating methods of different chemical forms for isotope analytical techniques will be developed. The aims of the study are more accurate quantitative detection of fossil, radioactive and biogenic carbon sources in the media mentioned before to survey the human pollution and improve understanding of temporal and spatial distribution of greenhouse gases in the atmosphere. In the framework of the investigation the accelerator mass spectrometry (AMS) gas ion source application will be introduced for the sample types mentioned above, to permit radiocarbon measurements in the range of 0.01-0.1 mg carbon. In addition to carbon-dioxide, laser spectroscopy methods (Cavity Ring-Down Spectroscopy) will be introduced in the laboratory for the stable isotope analysis of the atmospheric methane and carbon-monoxide.

Investigation of physical and chemical effects of ion irradiation on different materials and their possible applications

It is known that irradiation of materials with ionizing radiation is accompanied by radiation-induced effects, that is, changes of the chemical structure and/or physical properties. The basic processes in collisions of atoms and molecules with heavy charged particles are not fully understood yet. Besides their great importance in fundamental physics, these processes are important in many areas of science and applications. The final products formed during ion irradiation in a certain material depend on the formation and reactions of reactive intermediates such as excited states, ions and free radicals. However, it is not known yet how these reactions are affected by the characteristics of the irradiation source (i.e., the type of the particle, its energy and the linear energy transfer (LET)). Thus, the relation between the ion-molecule interactions (atomic collisions) and the subsequent physical and chemical effects are still not well understood, although it plays a very important role in space, medical and materials science or in ion beam therapy. Also, these processes are utilized in applications such as ion beam or electron lithography, development of new resist materials, creating micro and nano filters, microfluidic devices, among others. The PhD candidate will study the irradiations of different organic material (mostly polymers) and the subsequent physical and chemical effects, then utilizing the results in different applications.

Research and development of sensor principles, devices, sensor networks and IoT systems to monitor physical, environmental, industrial, transport, electricity and medical related processes

Digitization, the computer control of various processes has become decisive in many areas of life. Process control requires the collection of various information from the environment. Sensing, as the detection and measurement of environmental parameters, is necessary to develop an adequate response to the changes in the environment. The physical, chemical, biological, etc. signal is translated by the sensing device, the sensor converts it into a measurable, usually electrical signal.

The research and development of new types of sensors is based on first physical principles, materials science and technology.

It is also important to integrate the devices into sensor networks, in order to collect the required information from large space and time frame.

The development and application of new sensors is at the forefront of research and development in many areas, such as self-driving vehicles. It requires intelligent sensors that continuously monitor the environment and pre-process information even locally in the sensor device. The control of industrial processes and the application of robotics are also based on the data provided by the sensors. Smart homes and buildings, smart city, smart environment, as well as medical diagnostics or personalized medicine are important areas for the use of sensors.

Smart buildings will play an important role in the future operation of the electricity system. The flexibility they provide allows for a greater degree of integration of renewable energy sources into the electricity system. The use of ICT and IoT technologies will increase the operational security and flexibility of the electricity network. The combined use of these technologies is the first step towards the implementation of smart grids.

The research topic covers a wide range of research on the principles of perception, implementation, device development, and various sensory applications.

The task of the PhD student - together with the industrial partner - is to study the integration of smart buildings using renewable energy sources into the energy network, to perform the related network calculation, simulation and modeling tasks, to examine and qualify test systems.

Investigation of environmental effects in biological samples

It is well known that bone can be one of the final destinations in the body where toxic elements are deposited. Therefore we have a chance to identify and clarify various environmental effects in bones. The aim of the present work is to investigate the major and trace elements in bones measured by various physical methods. We focus on the study of minerals concentrations, crystallinity levels and surface properties of the bones. We plan to use Scanning Electron Microscope (SEM), Photoelectron Spectrometer (XPS), Fourier Transformed Infrared Spectroscopy (FTIR) and Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES).

Good skill of manuscript writing in English

Excitation of optically active nanocrystals and thin films with charged particles

As a response to external excitations some semiconducting materials produce strong luminescence due to their special electronic structure. An enhancement of the luminescence intensity can be observed when the emitter has a nanocrystalline structure, because transition probabilities drastically increased by the quantum size confinement effect. On the one hand, these materials are of practical importance, for example are used as light absorbing layers in solar cells, light emitting devices (LED), or radiation detectors. On the other hand, these materials essential for research purposes targeting a deeper understanding of fundamental processes primarily involving charge-carrier dynamics, damping and recombination mechanisms. Although there has been intensive research activity in the field of optoelectronic excitations of semiconductors, related phenomena have barely been observed for processes induced by charged-particle radiations. Basic energy transfer mechanisms by ionization can be well described in condensed matter, but their connection with the electronic transitions and luminescence behaviour of semiconductors is still an unexplored field.

The research work of the candidates will include the synthesis techniques of nanocrystalline materials, sample preparation, and characterization using electron microscopy and X-ray diffraction. They would be involved in a wide scale of irradiation experiments and optical measurements mainly at the Tandetron Laboratory of ATOMKI. The candidates may acquire a deeper knowledge on various measurement techniques, cutting-edge solutions of nuclear instrumentation, data analysis, the physical background of investigated phenomena, as well as can gain insight into several fields of modern physics as a participant of an interdisciplinary research.

Space radiation - mitigation and adaptation

The next decade will see humanity return to the Moon and the beginning of permanently crewed habitable structures in space. However space is a harsh environment and it is necessary to mitigate hazards such as stellar and cosmic radiation whilst adapting to the space environment. It is therefore necessary to not only protect humans going in space but to select and fabricate the materials with which to construct the structures within which humans and their equipment will operate.

Using the ion irradiation facilities at Atomki in this project we will explore the physical (and chemical) properties of materials needed for such architectures. This is materials science under space conditions. Materials include polymers, metallic composites and designed materials such as aerogels. Since transport of materials to the moon (and later Mars) is expensive we must use local resources such as lunar and Martian regoliths both as building materials and as a source of water, oxygen, ... etc, thus testing lunar and Martian regolith analogues will be important.

Simultaneously with such experimental studies it is necessary to develop a detailed space radiation code that can predict the physical (and chemical) changes induced by space radiation on materials. In collaboration with the MBN Research Centre at Frankfurt in a parallel PhD we will construct a radiation damage model that is based upon understanding of radiation damage at the atomic and molecular level leading to macroscale damage. Such a model is statistical in nature and requires inclusion of both quantum mechanical nature of atomic/molecular damage and a stochastic approach to the propagation of such damage to the macroscale. The final model should be predictive in nature in order to assign risk to structural failure (and biological effects).

V. Particle Physics program

Supervisor: **Dr. Gábor Dávid**

PF5/424-02

Neutral meson production in Au-Au collisions at RHIC

In the first year of data taking at the Relativistic Heavy Ion Collider a significant suppression of pizero production at high transverse momenta has been observed. This result is very different from what has been seen at lower energies (AGS, SPS) and it triggered a substantial amount of theoretical work. The candidate is expected to analyze the data from the second year of RHIC running, to extract the pizero and eta cross-sections up to the highest possible transverse momentum and compare the results to state-of-the-art theories. He/she is also expected to participate in data taking, calibration and general maintenance of the electromagnetic calorimeter of PHENIX.

Supervisor: **Dr. Gábor Dávid**

PF5/425-02

Sources of direct photons in heavy ion collisions at RHIC

Early results in relativistic heavy ion collisions at RHIC have shown that direct photon production scales with respect to p+p collisions as the number of binary nucleon-nucleon collisions. However, theoretical calculations and a closer look on data suggest that this scaling might be violated at all transverse momenta (p_T): by thermal production at low p_T , quark Bremsstrahlung and jet-photon conversion at medium p_T and the isospin-effect and/or modifications of the structure functions at high p_T . The candidate is expected to work on methods to disentangle the contributions from different sources (production mechanisms) to the direct photon spectrum using the electromagnetic calorimeter of the PHENIX detector. He/she is also expected to participate in data taking, calibration and general maintenance of the electromagnetic calorimeter of PHENIX and general software development for the experiment.

Supervisor: **Dr. Gábor Dávid**

PF5/426-02

Search for signatures of the Quark-Gluon Plasma in Au+Au collisions at RHIC

The first year of data taking at the Relativistic Heavy Ion Collider at Brookhaven provided many tantalizing results pointing towards the possible formation of a quark-gluon plasma in Au+Au collisions. However, these results do not form a coherent and convincing picture so far. There are many open questions both from the theoretical and from the experimental side. The candidate is expected to work on analysis methods that correlate different experimental signatures in order to confirm or to rule out theoretical scenarios with a higher confidence level. He/she is also expected to participate in data taking of the PHENIX experiment, contribute to the general and detector-specific software framework, and work on 2nd and 3d level trigger algorithms in order to facilitate data taking at the expected high luminosities.

Supervisor: **Dr. Zoltán Trócsányi**

PF5/428-02

Calculation of radiative corrections in perturbative QCD

The theoretical framework to describe the strong interaction of elementary particles is Quantum Chromodynamics (QCD). Due to the asymptotic freedom property of QCD the high-energy interactions can be described using perturbation theory. However, the large value of the strong coupling makes the leading order predictions rather imprecise. In order to make sufficiently precise theoretical predictions the inclusion of radiative corrections is imperative in for the most processes. The purpose of the research is to calculate radiative corrections to the phenomenologically most interesting processes (Higgs production, backgrounds for Higgs search, jet physics).

Supervisor: **Dr. Zoltán Trócsányi**

PF5/438-08

Searching for new particles with the CMS detector at the LHC

At the LHC, the energy of the most energetic elementary particle (parton-parton) collisions will be in the TeV energy range. As a result, the most exciting new “particle” that may appear at the LHC is a microscopic black hole. Some of the collisions that occur at larger energy than the $(4+n)$ -dimensional Planck-scale can be viewed as $(4+n)$ -dimensional gravitational interaction. There are numerical simulations in the literature which predict that the production of microscopic black holes in such cases is large. As a result of Hawking radiation, such a black hole will decay immediately into many different particles of the Standard Model. Studying the final state of such an event, we can draw conclusion about the number of extra dimensions. Although, the current theoretical understanding of the process is rather vague, event generators, that can be used to study the proton-proton collisions which lead to black holes, exist. The goal of this research is to search for particles in events at the LHC that would indicate the existence of extra dimensions.

Supervisor: **Dr. Zsolt Schram**

PF5/439-08

Topological excitations and quark confinement

Topological excitations as magnetic monopoles or vortices play an important role in forming the phase structure of lattice gauge theories and in quark confinement. This has been shown in analytic and numeric studies for the $U(1)$ model. Non-abelian gauge theories, however, still pose a number of open questions. Within this project we study numerically the vortex model of confinement using lattice field theoretical methods. First we examine the physical properties of vortices in the simplest, $SU(2)$ model, in $D=2+1$ dimensions. Most important questions are, how one can identify vortices on a lattice and what the physical characteristics of the identified vortex configurations are. We examine the possible connection between vortices and abelian monopoles regarding confinement. We generalize our studies for $D=3+1$ dimensions and for the physically more interesting $SU(3)$ case.

Supervisor: **Dr. Dezső Horváth**

PF5/440-10

Test of the equivalence of matter and antimatter at the Antiproton Decelerator of CERN

One of the mysteries of physics is why there are no antimatter galaxies in the Universe, why antimatter disappeared after the Big Bang. The Antiproton Decelerator of CERN was built in 2000 to test the principle of CPT invariance stating the equivalence of matter and antimatter. The ASACUSA Collaboration of Japanese, Austrian, Danish, German, Hungarian and Italian groups studies in several different experiments the properties of antiprotons: measuring the mass and magnetic moment of the antiproton in antiprotonic helium atoms using high-precision laser spectroscopy. and prepares an experimental apparatus for the spectroscopy of antihydrogen in electromagnetic traps. The doctoral student should join these studies following the earlier Hungarian students. The Hungarian participation is supported by the OTKA grant K72172.

Supervisor: **Dr. István Nándori**

PF5/441-11

Renormalization group method and phase transitions

The renormalization group (RG) method is one of the most effective and most dynamically evolving branch of modern physics. The method enables us to eliminate the quantum fluctuations systematically in physical models giving us its low energy, effective behaviour. The effective theory can account for the phase structure of the model. The description of the symmetric phase is well known in the literature. However the effective theory in the broken symmetric phase cannot be determined easily, because the RG evolution equation is singular there. The problem can only be treated if we choose such a renormalization scheme where the singularity is manageable. On the one hand there are cases when the singularity does not even turn up for certain renormalization schemes. On the other hand one can assume that there is an infrared fixed point, where the couplings show relevant scaling. Then the evolution of the couplings can be calculated arbitrarily close to the singularity.

Our goal is to determine the scaling of the couplings of scalar field theoretical models in the vicinity of the fixed point of the broken symmetric phase. We intend to study the low energy effective behaviour of the models and calculate the critical exponents characterizing the phase transition. This requires the inclusion of the wave function renormalization, which can be taken into account self-consistently in the framework of RG method.

Supervisor: **Dr. Kornél Sailer, Dr. Sándor Nagy**

PF5/442-12

Functional renormalization group for open quantum systems

The main goal is to study nonequilibrium physics of simple, open quantum systems in quantum field-theoretic framework. It can be investigated the decoherence of a coherent superposition of quantum states due to the influence of environmental effects, the possibility of a phase transition with varying strength to the environment or the temperature of the environment, and open quantum systems showing up dissipative quantum chaos.

There are a lot of important, experimentally realizable simple quantum systems which can be modelled by quantum Brownian motion: a particle moving under the exertion of an external force and coupled to the environment. Following Caldeira and Leggett the environment can be reliably modelled by either a zero-temperature or a finite temperature system of an infinite set of independent harmonic oscillators. The functional renormalization group method enables one, on the one hand to treat the nonperturbative behaviour of the particle moving under the exertion of the external force (e.g. that of the anharmonic oscillator) and, on the other hand, to study the case of strong coupling of the particle to the environment. The model outlined above offers the possibility to investigate the transition from quantum to classical physics. Aiming this one has the possibility to study the effect of the thermal and quantum fluctuations on the decoherence. The systematic treatment of any fluctuations can be performed by the functional renormalization group method. With varying coupling to and temperature of the environment one expects that a new, broken symmetric phase appears in the model. We assume that there is an infrared fixed point in this phase, where the scaling properties of the model change. The fixed point enables us to determine the flow of the couplings around the singularity. We intend to study the phases of the model, and their critical exponents. This requires the inclusion of the wave function renormalization, which can be taken into account self-consistently in the framework of RG method.

Supervisor: **Dr. Tamás György Kovács**

PF5/443-13

Quantum-chromodynamics on the lattice

Quantum-chromodynamics is the generally accepted theory describing strongly interacting matter. Recently we found that at high temperature, in the so called quark-gluon plasma state, the lowest quark states become spatially localized. This phenomenon is analogous to the localization of electron states in imperfect crystals, known as Anderson localization. We would like to study the nature of these localized quark states and the transition in the spectrum from localized to delocalized states.

Supervisor: **Dr. Viktor Veszprémi**

PF5/444-14

Search for supersymmetric particles using the CMS detector at the Large Hadron Collider

The Large Hadron Collider (LHC) located at CERN is the largest particle accelerator in the World since its start-up in 2009. It produces new particles through microscopic explosions induced by colliding protons. The distribution and properties of these particles carry information on the basic laws that govern the interactions between the fundamental building blocks of the matter. The goal of the LHC is to determine the exact properties of the Higgs boson and to discover signs of physics beyond the Standard Model (SM), the most successful comprehensive theory of particle physics so far. An example for such an extension to the SM is the theory of supersymmetry (SUSY). The accelerator is under a continuous development in order to make it produce collisions at higher and higher energies and rate. The next running period of the LHC starting in January 2015 might be the most important one.

The Compact Muon Solenoid (CMS) is a multi-purpose detector that was developed in order to perform searches for new physics. Hungarian scientists have been participating in the construction and operation of the CMS for nearly two decades. Our present goal includes the upgrade of the CMS charged particle tracking system (the Pixel detector) in order to meet the challenges posed by the LHC upgrades, as well as finding evidences for particles predicted by supersymmetric models in the data recorded by the CMS detector. The CMS tracking system plays a fundamental role in the detection of particles potentially created by supersymmetric processes. The successful candidate will have the opportunity to work with colleagues from the Wigner Research Centre for Physics and the Swiss Paul Scherrer Institute, as well as to make frequent visits to CERN.

Supervisor: **Dr. Gábor Somogyi**

PF5/445-15

Describing elementary particle collisions with high precision

The observation and theoretical interpretation of high energy elementary particle collisions is a very important tool for understanding the nature of physical laws at the subatomic scale. The high precision of experimental measurements at the Large Hadron Collider for basic processes – such as the production of jets, heavy quarks, the Higgs-boson or vector bosons – demands that the computed theory predictions be similarly precise. In order to reduce the theoretical uncertainty it is useful and in some cases necessary to compute radiative corrections in quantum chromodynamics to next-to-next-to-leading order accuracy. The proposed research topic is the computation of these radiative corrections to processes of basic phenomenological importance.

Supervisor: **Dr. Sándor Nagy**

PF5/446-15

Functional renormalization group method in quantum theories

Our goal is apply the functional renormalization group (RG) method in quantum field theoretical models. The RG method is widely used in many branches of modern physics. It is mainly used for describing the phase structure of the investigated models. We start from the high energy action of the physical system and we look for its low energy behavior. We use the path integral form of quantum field theory, where the path integral itself contains all the paths which are between the given initial and final states. The deviations of the paths from the classical trajectories appear as quantum fluctuations or degrees of freedom in the theory. They should be systematically taken into account if we want to determine some physical quantities. The RG method provides us a suitable tool to handle this problem. The method gives a partial differential equation for the effective action, which is known as the Wetterich equation. From the equation the (energy) scale dependence of the couplings can be calculated, which characterize the corresponding interaction. The scale dependence can provide us the phase structure, the low energy behavior or even the appearing decoherence in the investigated model. The RG method will be used in scalar models (e.g. in the d-dimensional $O(N)$ model, in the sine-Gordon model), in gauge theories (e.g. in quantum electrodynamics) or in quantum Einstein gravity.

Supervisor: **Dr. Zsolt Schram**

PF5/447-15

Thermodynamics in non-abelian lattice gauge theories

In high energy heavy-ion collisions formation of a new phase of matter, the quark-gluon plasma is expected. For non-abelian gauge fields calculations based on the grand canonical ensemble showed the existence of a deconfining phase transition at finite temperature. However, clearly the application of the grand canonical ensemble at zero baryon density is a strong simplification. Calculations at finite baryon density has been done recently, but these are difficult and there are still a number of questions to answer. In our work we carry out lattice studies in various gauge theories using a new method where, instead of the usual (grand) canonical distribution, we implement in the simulations the so-called Tsallis distribution which shows power-like characteristics at higher energies. This novel approach can be formally interpreted as calculating expectation values of observables over fluctuating temperature. In our case the temperature fluctuates with a Gamma distribution. Our aim is to explore the phase structure of the systems under consideration and to determine the corresponding equations of state.

Supervisor: **Dr. István Nandori**

PF5/448-16

Compactness, differentiability and renormalization

The construction of models in Quantum Field Theory is based on classical symmetry principles. Subsequent quantization and the relativistic description result in scale-dependent parameters, which require renormalization. Thus, in order to obtain measurable quantities and to construct the low-energy effective theory of the corresponding microscopic model, one has to perform renormalization.

In models of gravity in large extra dimensions, like the Randall-Sundrum (RS) theory, the extra dimensional space is compact similarly to field theories suitable for the description of vortex dynamics in layered superconductors. Moreover, in the RS theory the effective model for branon-fluctuations contains the modulus of the field similarly to the $O(N)$ symmetric sine-Gordon model, so non-differentiable potentials emerge. The goal of the present research project is to investigate the effect of compactness and differentiability on renormalization in the framework of functional renormalization group.

Supervisor: **Dr. Balázs Ujvári**

PF5/449-16

Simulation of the experiment measuring the weight of the neutrino

The candidate will continue the simulation of the recommended experimental setup (U.D. Jentschura, D. Horvath, S. Nagy, I. Nandori, Z. Trocsanyi, B. Ujvari, Int.J.Mod.Phys. E23 (2014) 1450004). The accelerated particle beam, the interaction with the target, the secondary particles, their decays, the detection of the neutrino, the electronics and the data acquisition has to be simulated in GEANT4 framework. The parameters like length, energy of the beam, the width of the target, the magnetic field has to be optimized. With the modern data analysis techniques the candidate will set the limit for the mass of the neutrino. It is

important to gain experience with the latest detection and acceleration techniques to implement in the future available solutions in the simulation.

Supervisor: **Dr. Balázs Ujvári**

PF5/450-16

Hardware development in particle physics

There are two main topics:

1. The sPHENIX (starting operation in 2021) electromagnetic calorimeter will use silicon photomultipliers (SiPMs) in the electromagnetic calorimeter. An automated test equipment will be needed to measure the gain dependence on temperature, bias voltage and the radiation damage. The SiPM output will be digitalised, this module will create the trigger primitives. The trigger signal will be based on these primitives. The candidate will help the work of the trigger group by preparing simulations of the performance of SiPMs. Using the parameters, based on the simulations, the next step is the planning and the construction of the FPGA based trigger electronics prototype.
2. Simulation of the radiation hardness and test of the CMS Muon Endcap system front-end and read-out electronic modules.

The candidate will participate also in the preparation of the readout system and an algorithm of a multiwire proportional chamber for detecting cosmic muons. This device will be used in physics student laboratories at the department.

Supervisor: **Dr. Ádám Kardos**

PF5/451-18

Developing a numerical framework to compute radiative corrections in Quantum Chromodynamics

Radiative corrections in Quantum Chromodynamics are of key importance for the Large Hadron Collider (LHC) in order to interpret the results of measurements precisely. Computing such corrections is mandatory for precision tests of the standard model and in search of new physics beyond it. Currently the state of the art is the computation of second radiative corrections in QCD for which yet so far there exist no general framework that is satisfactory for all expectations. The task of the student will be to contribute to the development of such a framework and afterwards implementing and obtaining radiative corrections for key processes for LHC experiments.

Supervisor: **Dr. Balázs Ujvári**

PF5/452-19

Direct photon production in Au+Au collisions

It is well established that in ultrarelativistic heavy ion collisions a new form of matter, the Quark-Gluon Plasma (QGP) is formed. Properties of the QGP have been studied both at RHIC and at LHC. Direct photons are produced during the entire space-time evolution of the QGP and they are the only known penetrating probes, carrying direct information on the entire history of the collision. The candidate will analyze the combined 2014-2016 200 GeV Au+Au dataset taken by the PHENIX experiment at RHIC. These data represent about 15 times the statistics of earlier publications, and their analysis is expected to provide the final, archival result on photons at 200GeV, with large improvement on statistical and systematic uncertainties, extended transverse momentum range, and direct impact on pQCD calculations, nuclear PDFs and possible modification of fragmentation functions, understanding of collision geometry and the jet energy scale.

Supervisor: **Dr. Balázs Ujvári**

PF5/453-19

Neutral meson production in 200 GeV Au+Au collisions

It is well established that in ultrarelativistic heavy ion collisions a new form of matter, the Quark-Gluon Plasma (QGP) is formed. Properties of the QGP have been studied both at RHIC and at LHC. High transverse momentum neutral mesons, in specific π^0 and η , are produced as leading particles of jets originating from a parton that underwent initial hard scattering then traversed the QGP and lost energy in it. Measuring the energy loss via the nuclear modification factor of π^0 and η , including its azimuthal variation with respect to the reaction plane of the collision provides crucial information on the properties of the QGP. The candidate will analyze the combined 2014-2016 200 GeV Au+Au dataset taken by the PHENIX experiment at RHIC, These data represent about 15 times the statistics of earlier publications, and their analysis is expected to provide the final, archival result on π^0 and η at 200GeV, with large improvement on statistical and systematic uncertainties, extended transverse momentum range, and direct impact on theoretical models of parton energy loss in the QGP, the possible flavor dependence of the energy loss.

Supervisor: **Dr. Gábor Dávid**

PF5/454-21

Simulation techniques in particle physics and search for η , K^0_S and ω mesons in 200 GeV Au+Au collisions in the PHENIX experiment at RHIC

The measurement of hadrons produced at high transverse momenta (p_T) is a well established tool in the study of the hot and dense medium produced in relativistic heavy ion collisions. The highest p_T has been reached so far with the lightest hadron (π^0), but the high statistics Run-14 and Run-16 Au+Au data set at 200 GeV of the PHENIX experiment at RHIC

makes it possible to extend the measurement to heavier hadrons (ω) and also hadrons with hidden or open strangeness (η and K^0_S). Establishing the suppression of these heavy hadrons or lack thereof will give important additional information of the parton energy loss in the medium, as well as on possible differences between the energy loss mechanism of light (u,d) and heavier (s) quarks. We will study the η production in the $\eta \rightarrow \gamma \gamma$ decay channel, ω production in the $\pi^0 \gamma$, and, if feasible, production in the $K^0_S \rightarrow \pi^0 \pi^0$ decay channels. In several steps of the analyses we will use the GEANT3 simulation framework of PHENIX. Also, by comparing to testbeam results, we will verify the GEANT4 simulation of the BTL subdetector of CMS (LHC), and integrate it into the general simulation framework of CMS.