PhD26-24

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

2026.

Director: Prof. Dr. Ferenc Kun

University of Debrecen, Faculty of Science and Technology,
Department of Theoretical Physics
Address: H-4026 Debrecen, Bem tér 18/b, Hungary
Postal address: H-4002 Debrecen, POBox 400, Hungary
Phone: +36-52-509-201, Fax: +36-52-509-258
E-mail: ferenc.kun@science.unideb.hu
URL: http://physphd.unideb.hu

Edited by:
Dr. László Oláh

Table of Contents

Debrecen, March 2026

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 emphasise 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 Tőkési** **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 resodnance (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 $\eta = Q/v >> 1$ (*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, $n>>1$ 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 measurments 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 dinamics

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 movingheavy 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. 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 tremperature. 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. Kinematicaly 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 in 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).

Supervisor: **Dr. Erika Bene** **PF1/444-19**

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 avaliable such as quantum computers, quantum simulators, and secure quantum communication. Quantum informatics may hold the key for a technological revolation. 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.

Supervisor: **Dr. Tamás Vértesi** **PF1/445-19**

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.

Supervisor: **Dr. Károly Tőkési** **PF1/446-19**

Modelling of atomic processes in fusion plasma

The recently used energy production methods will not be able to saisfy 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 ofthe best solutions in fuhue 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 ofthe ions in ion-atom and ion-surface collisions and the fusion chamber damage during ion irradiation. Specifically, we look for the answers 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 section sections for H, D, T, H^+, D^+, T^+ projectiles. To make the calculations. we will usc the different versions of the classic Monte Carlo and quantum mechanical methods.

(b) Along the plan a) we determine the energy and angular diflerential 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 programing language (Fortran, C, C++, etc).
Good skill of manuscript writing in English.

Supervisor: **Dr. Andrea Orbán** **PF1/447-19**

Ultracold molecular gases

The proposed research topic is related to the rapidly growing research field of ultracold
(< 1 μK) quantum gases. Such systems are expected to play major role in future quantum technologies, which is one of the flagship project 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 super-conductivity 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 jet 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 39K133Cs 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

ATOMKI's instrumentation (ECR, Tandetron ion accelerators and infrared spectrometers) and the 2 facilities built in a Hungarian-British collaboration for the production and analysis of thin ice layers (Ice Chamber for Astrophysics/Astrochemistry, Atomki-Queen's University Ice Laboratory for Astrochemistry) allow us to study the physical and chemical changes of interplanetary ices under the influence of ion and electron irradiation. During these processes, complex organic molecules are created, which will be studied in the near future by various space missions. Experiments on Earth are also needed to interpret the data from space probes. The accelerators cover almost the entire range of ion energies of the solar wind and cosmic rays, whose effects can thus be studied. In addition to ices, other solid materials can also be studied. The student will be responsible for carrying out experiments to investigate an astrophysical problem of his/her choice, interpreting the data and publishing them.

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 Tőkési** **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 eletronic 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 programing language (Fortran, C, C++ etc).
Good skill of manuscript writing in English The recently

Supervisor: **Dr. Zsolt Mezei** **PF1/452-21**

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 intricated 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 (CH4) and acetylene (C2H2) 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 C2H 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.

References:

[1] Tielens A.G.G.M, Rev. Mod. Phys. 85, 1021 (2013);
[2] Mezei J.Zs. et al., ACS Earth Space Chem. 3, 2367 (2019);
[3] Sciamma-O'Brien E. et al., Icarus 209, 704 (2010);
[4] Mikikian M., et al., Plasma Phys. Control. Fusion 59, 014034 (2017);
[5] Hassouni K., et al., J. Phys. D: Appl. Phys. 43, 153001 (2010);
[6] Tennyson J., Phys. Rep. 491, 29 (2010)

Supervisor: **Dr. István Márton** **PF1/453-23**

Semi-device-independent EPR steering scenario with many measurements and multi-component systems

Randomness is a resource for cryptographic applications, numerical algorithms and simulations. However, standard methods for generating randomness rely on assumptions about the devices that are often unsatisfactory in practical situations. Quantum technology, on the other hand, is a new class of technology that allows for a more efficient manipulation of information. In particular, it enables new methods for generating certified randomness based on violations of Bell inequalities. These methods are called device-independent because they do not rely on any modelling of the devices. Our goal in this research is to understand and explore the new possibilities offered by semi-device independent quantum random number generator scenarios. The key idea here is to keep some of the device-independent spirit and make only mild assumptions about the configuration, but without detailed modelling of the devices. The hope is that the hardware requirements for implementing semi-device independent scenarios will be not as high as those for the device-independent scenario. In this project, the PhD student will contribute to the development of the theoretical and numerical background for the implementation of a semi-device independent quantum random number generator. In particular, in addition to the bipartite setup, the multipartite setup will be investigated, where the phenomenon of cyclic EPR correlations has recently been observed. One of the main goals is to answer the question whether correlations exhibiting the cyclic EPR-steering phenomenon can help to reduce the critical detection efficiency parameter and thus contribute to the technological implementation of semi-independent quantum random number generators.

Supervisor: **Dr. Sándor Demes** **PF1/454-24**

Study of astrochemically relevant molecular interactions using robust quantum chemistry and molecular scattering methods

A better understanding of the physico-chemical conditions in the molecular clouds of the interstellar medium is essential for understanding the life cycle of matter in space, in particular the formation of stars and planets and the synthesis of complex organic molecules. In extreme astronomical environments, radiative and collisional processes compete with each ther to populate the molecular levels. A detailed understanding of such state-selective processes is therefore of key interest to observational astronomy, but also has strong interdisciplinary relevance in different fields of physics and chemistry.

The project aims to investigate the interaction potential and collision dynamics between complex interstellar molecules and the most common collision partners in space (H_2, He, H). To this end, we will develop multidimensional potential energy surfaces using accurate quantum chemical methods. Following a proper analytical fit of these potentials, we will perform collisional dynamics calculations using exact quantum-mechanical and semi-classical scattering theories, which will require mostly new methodological developments. In the final phase of the work, we will calculate rotationally and vibrationally state-selective cross sections and thermal rate coefficients for the collisions of key astrochemical molecules.

These will also be incorporated into radiative transfer models that will allow the simulation of astronomical observations made by the advanced telescopes, such as JWST, ALMA, GBT, Yebes, IRAM, etc.

The project is recommended for candidates interested in molecular physics, physical chemistry, astrophysics and space chemistry. They should have a basic knowledge of quantum mechanics and molecular spectroscopy, and an affinity to perform large-scale numerical computations, chemical simulations, as well as methodological and code development. They will also have the unique opportunity to use the most powerful High Performance Computing (HPC) facility in Hungary, the Komondor.

Supervisor: **Dr. Andrea Orbán** **PF1/455-25**

Optical shielding of ultracold ion-atom collision

The proposed research topic is related to the quantum physics of dilute gases at ultracold (< 1μK) regime. In the last decades impressive experimental results have been obtained thank to the progress in the laser cooling and trapping techniques of neutral and charged particles (Nobel Prizes in Physics in 1997, 2001) in parallel with outstanding theoretical developments to model such novel quantum matter. Meanwhile laser cooling techniques were also applied to trap atomic ions at low temperatures too, well below 1 Kelvin (Nobel Prize 2012). The idea of merging these two techniques, i.e. putting together cold atoms and ions, came up in many research groups around the world leading to the realization of the so-called hybrid traps. Such systems appear as amazing platforms to study ion-neutral interactions and ultracold chemistry, many-body quantum physics, and to explore ways toward quantum simulation of condensed matter and quantum information protocols.

A challenging contemporary goal regarding reactive processes is to obtain high level control and selectivity, resulting controlled reaction pathways and reaction products, a domain now identified as ultracold chemistry. In several experiments (e.g. [1, 2]), a single ground state ion is embedded in a dense cloud of ultracold ground state atoms close to quantum degeneracy. The ion then acts as an impurity for the ultracold gas. Due to the strong long-range charge induced dipole interaction varying as R^{-4}, compared to the weak atom-atom R^{-6} interaction, the probability for three-body events becomes dominant in degenerate gases [2], leading to unwanted losses, e.g. by resulting to the creation of molecular ions. In the context of future applications for quantum many-body physics, these losses are unwanted. To prevent such ion-losses, in the proposed theoretical work, we will consider the possibility of the optical shielding (OS) [3, 4] of short-range ion-atom physics by engineering the long-range interaction between the ion and the atom using a laser tuned to the blue of an optical transition in the atom. The principle is to couple with light the attractive entrance channel of the collision to a repulsive channel at large distances, so that the colliding particles are indeed reflected back without reaching the short-range reaction zone. We will focus on Li-Ba+ system [1], [5] as it presents the interesting feature of being completely protected against non-radiative charge exchange: indeed, the entrance channel of two colliding ground state particles is the actual ground state of the system, usually in contrast to other combinations of alkali-metal atom and alkaline-earth ion systems. As a first step we will extend our methodology developed for the OS between two neutral atoms of different species [4]. The OS scheme will be based on the repulsive long-range potential energy curves correlated to the Ba+(6s) + Li(2p) asymptote: the OS laser will then be tuned to the blue of the 2s -> 2p transition of Li. The main limitation of such a one-photon optical shielding is the heating of the quantum gas due to the continuous scattering of off-resonant photons of the shielding laser.

Therefore, in a second step we will extend the two-photon optical shielding scheme which has been proposed to shield molecule-molecule collision [6]. The implementation of the one/two-photon OS necessitate to consider the complexity of states (fine and hyperfine structure) involved in the shielding scheme, thus high-level molecular structure calculations have to be performed. This will be followed by the low energy collision dynamics treated with quantum coupled channel method.

[1] P. Weckesser, F. Thielemann, D. Wiater, A. Wojciechowska, L. Karpa, K. Jachymski, M. Tomza, T. Walker, and T. Schaetz. Observation of Feshbach resonances between a single ion and ultracold atoms. Nature, 600, 429, 2021.

[2] A. Mohammadi, A. Krükow, A. Mahdian, M. Deis, J. Pérez-Ríos, H. da Silva, M. Raoult, O. Dulieu, and J. H. Denschlag. Life and death of a cold BaRb+ molecule inside an ultracold cloud of Rb atoms. Phys. Rev. Res., 3, 013196, 2021.

[3] T. Xie, M. Lepers, R. Vexiau, A. Orbán, O. Dulieu, and N. Bouloufa-Maafa. Optical shielding of destructive chemical reactions between ultracold ground-state NaRb molecules. Phys. Rev. Lett., 125, 153202, 2020.

[4] T. Xie, A. Orbán, X. Xing, E. Luc-Koenig, R. Vexiau, O. Dulieu, and N. Bouloufa-Maafa. Engineering long-range interactions between ultracold atoms with light, J. Phys. B, 55, 034001, 2022.

[5] X. Xing, P. Weckesser, F. Thielemann, T. Jónás, R. Vexiau, N. Bouloufa-Maafa, E. Luc-Koenig, K.W. Madison, A. Orbán, T. Xie, T. Schaetz, and O. Dulieu. Competing excitation quenching and charge exchange in ultracold Li-Ba+ collisions. J. Phys. B, 57, 245201, 2024.

[6] C. Karam, R. Vexiau, N. Bouloufa-Maafa, O. Dulieu, M. Lepers, M. Meyer zum Alten Borgloh, S. Ospelkaus, and L.Karpa. Two-photon optical shielding of collisions between ultracold polar molecules. Phys. Rev. Res., 5, 033074, 2023

II. Nuclear Physics program

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...

Supervisor: **Dr. Barna Nyakó, Dr. István Kuti** **PF2/413a-b-93**

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 symultaneous 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»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»130,150 and A»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 appearence 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»150 and A»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»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. Ferenc Ditrói** **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. János Gál** **PF2/427-96**

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.

Supervisor: **Dr. Géza Lévai** **PF2/428-96**

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. 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 appearence 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. 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?](>2Ď€), good energy (1%) and angular (2º) 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 emittion. 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. 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).

Supervisor: **Dr. Zoltán Elekes** **PF2/454-13**

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 reasearch institues: RIKEN (Japan), GSI (Germany), GANIL (France).

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 led 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, word 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 shieling 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 Csedreki** **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.

Supervisor: **Dr. Andrea Ilona Furka** **PF2/460-22**

Evaulation of novel techniques in radiotherapy

Radiotherapy, as the fundamental part of Oncology, has undergone a very fast techniqal development. Novel techniques result longer overal 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 continous consultation with medical physicists.
Improvement in planning system and self-controlling methods may lead better quality therefore more radical radiotherapy, suggesting favourable clinical outcome.

Supervisor: **Dr. Karoly Osvay , Dr. Zsolt Fülöp** **PF2/461-22**

Optimisation of the yield of laser generated neutrons

Acceleration of charged particles with lasers have been continously 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.

Supervisor: **Dr. Alejandro Algora** **PF2/462-24**

Systematic investigation of Beta decay to answer nuclear structural and astrophysical questions

Beta decay is the most general form of element transmutation in the nuclide chart. As such, it can provide relevant information for nuclear structure, nuclear astrophysics and practical applications. In this framework, we propose a topic of research to perform a PhD thesis based on the study the beta decay of very exotic nuclei in both the neutron rich and proton rich sides of the nuclide chart using state of the art instrumentation. The experiments to be analyzed were/will be performed at the RIKEN facility using a high purity germanium array, a Total Absorption Spectrometer and neutron counters.
The proposed work is based on high quality decay data obtained in experiments performed at a very competitive international facility. The work implies the analysis of these complex experiments, and requires the development of analysis tools using Root and C++, the interpretation of the results in collaboration with nuclear and astrophysics experts and the publication of the results in high ranking journals.

Supervisor: **Dr. László Csedreki** **PF2/463-25**

Performance tests and applications of modern neutron sources

Due to the nuclear properties of neutrons, their study and applications play a crucial role in many fields of physics, e.g. understanding the nucleosynthesis of heavy elements, theory and applications of energy generation in nuclear reactions, material science and applications of neutron in medicine and health science.
The main feature of HUN-REN Atomki is characterized by charged particle accelerators, radioactive sources and nuclear experimental apparatus (gamma-, neutron- and charged particle detectors, nuclear electronics, etc.) provides to keep the leading role of the institute on the field of nuclear physics.
The main task of the PhD applicant will be concentrated on nuclear physics experiments involving the study and application of neutrons. The preparation and the planning of the experiments including the installation of new neutron sources, performing the measurements (target preparation and characterisation, in-beam spectroscopy and activation technique) and the analysis of data will be in the focus of the candidate carried out mostly at the HUN-REN ATOMKI experimental apparatus.

III. Solid State Physics and Material Science program

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. 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. Schadsehneider, Phys. Rev. Lett. 75(1995)4298. A. Korepin et al., Phys. Rev. Lett. 74(1995)789.

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 havy-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 ³ 1 dimensions in order to obtain main information connected to its physical behaviour. As a starting point we would like to use the method perfectioned 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 signiture 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 cathegory). 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. 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 cicumstances will be investigated by experimental methods in different (Ti-Ni, Cu-Zn-Al) shape memory materials.

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 explicite 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. István Csarnovics** **PF3/436-02**

Photostimulated processes in semiconductor nanostructures

Photostimulated structural transformations in light-sensitive chalkogenides and their influence on the optical, electrical parametres 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. István Csarnovics** **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.

Superrvisor: **Dr. István Csarnovics** **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. Ferenc Kun** **PF3/444-06**

Study of fractures and fragmentation processes in solid states

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 Daróczi** **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 Cserháti** **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, cilindrical, 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 methodes 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, tdudies by light and electron microscopes as well as X-ray diffraction.

Supervisor: **Dr. Ákos Nemcsics** **PF3/458-17**

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, doulbe-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-eptaxy. 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: evalutation 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, konowlwdge of English, practical sense (in the case of experimental works).

Superrvisor: **Dr. István Csarnovics** **PF3/460-19**

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.

Supervisor: **Dr. István Csarnovics** **PF3/461-19**

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. Viktor Takáts** **PF3/463-20**

XPS-LEIS measurement techniqes 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 Tőkési** **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 programing language (Fortran, C, C++ etc).

Good skill of manuscript writing in English

Supervisor: **Dr. Gábor Battistig** **PF3/467-23**

Development of material testing methods

The aim of the research is to implement material testing methods, develop and test the electronic equipment required for measurements and demonstrate their practical applicability. In materials science, in addition to traditional measurement techniques, there is an ever-increasing demand for the implementation of new procedures related to size reduction. In the examination of magnetic materials, it is no longer possible to follow the microstructural changes or to examine the interactions taking place between thin layers of very small mass using traditional techniques developed for bulk materials, often with large instruments.

During the doctoral work, the student investigates magnetic and/or thermal measurement technologies, their advantages and disadvantages, as well as the construction of measuring equipment. The goal is to develop measuring devices that meet emerging needs, relying on theoretical material science and electronics knowledge. After building the measuring equipment, demonstrate the practical applicability of the equipment with test measurements and calibration.

Qualifications of the applicant: degree in electrical engineering or physics or materials science, proficiency in measurement technology and designing and building electronics, knowledge of English language

Supervisor: **Dr. László Zoltán Tóth** **PF3/468-25**

Superelastic Behaviour of Shape Memory Alloys Studied by Acoustic Emission

Shape memory alloys (SMAs) such as NiTi and NiFeGaCo exhibit unique functional properties arising from reversible martensitic transformations, including the shape memory effect and superelasticity. In recent years, attention has turned to the so-called strain-glass state, in which atomic-scale disorder suppresses the long-range martensitic transition, leading to glass-like mechanical responses that nevertheless retain features of superelasticity. Understanding these complex behaviours requires techniques capable of capturing the underlying micro-mechanical processes in real time.

This PhD project aims to investigate the superelastic and strain-glass behaviour of several metallic SMAs through acoustic emission (AE) monitoring during mechanical loading. Tensile and compressive deformation tests will be performed using a universal testing machine while simultaneously recording AE signals to detect transient events associated with phase transformation, variant reorientation, and dislocation activity. Advanced data-analysis and signal-processing methods—including statistical and pattern-recognition approaches—will be applied to identify characteristic AE signatures corresponding to different transformation mechanisms and to distinguish between conventional superelastic and strain-glass responses.

The research will include preparation and testing of selected alloy compositions, evaluation of stress–strain behaviour and AE activity, and complementary characterization of microstructural changes by standard techniques such as X-ray diffraction or differential scanning calorimetry when available. The combination of acoustic emission with mechanical testing and modern data-analysis is expected to provide new insights into the kinetics and dynamics of martensitic transformations and disorder-driven strain-glass states.

The outcomes of the project will contribute to a deeper understanding of the fundamental mechanisms governing the functional properties of SMAs and may support the design of materials with improved fatigue resistance and stability. The precise focus and methodology will remain flexible and will evolve according to the experimental results obtained during the study.

Supervisor: **Dr. Lajos Daróczi** **PF3/469-25**

Investigation of the noisy character of structural transformations in steels

Many of structural changes in materials has intermittent cheracter. Classical examples are the magnetization processes in ferromagnetic materials and the martensitic transformations. In these cases, the discontinuous processes result magnetic (Barkhausen) and acoustic noises. In case of ferromagnetic martensitic materials both of the above mentioned processes can be observed. Plastic deformations, oxidation processes, etc. can be also sources of acoustic noises. The noise detection and analysis can be a very sensitive and effective method of the investigation of structural changes in wide range of materials.

Iron based alloys play determining role in industrial applications. The martensitic transformation in these systems results outstanding properties. In Fe Mn TRIP/TWIP (TRansformation Induced Plasticity/TWinning Induced Plasticity) steels have high strength, high toughness and formability because of the non-thermoelastic martensitic transformation. The details of the plastic deformation mechanisms in these alloys are not fully understood, because of the complexity of the microstructure. Dislocation slipping, twinning, strain-induced martensitic transformations are the most important processes during the plastic shape change. In other systems, like FeNiCoTi, FeNiAl or FePt thermoelastic, martensitic transformation can be observed. During the transformation the motion of interfaces (especially twin boundaries) has an intermittent character. Some of the above mentioned systems are ferromagnetic or ferromagnetic phases can be produced during the plastic deformation and/or phase transformation.

All of the above mentioned elementary processes are potential acoustic emission (AE) sources. The advanced AE analysis methods make possible the separation of different noise sources and combined by other methods like microscopy, DSC, magnetic emission, etc. help the better understanding the mechanism of the plastic deformation and martensitic transformations.

IV. Physical Methods in Interdisciplinary Researches program

Supervisor: **Dr. Zita Szikszai** **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 ^{3}H, ^{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.

Supervisor: **Dr. István Csige** **PF4/421-02**

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.

Supervisor: **Dr. László Palcsu** **PF4/427-08**

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 spaleothem 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.

Supervisor: **Dr. Imre Uzonyi** **PF4/429-08**

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, Rutherfold 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□1 □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 CO_2 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 CO_2. The candidate has to investigate the possibility to apply carbon-monoxide (CO) as a quantitative proxy for fossil fuel CO_2 in the atmosphere in this region using a high precision on-line monitoring system, developed in this work. The representativeness of tree ring ^{14}C 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-Puszta and Hegyhátsál in Hungary) where continuous observations of CO_2 mixing ratio was made in the past it will be possible to reconstruct the atmospheric fossil fuel CO_2 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.

Supervisor: **Dr. András Fenyvesi** **PF4/433-10**

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.

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 palaeoclimatological and isotope hydrological methods

Our research is based on the sensitive and precise analytical skills that we have been adopted in our institute in recent decades. We would like to continue to develop these methods, which will be then applied in isotope-hydrological and palaeoclimatological research. Our plans include the following topics:

- Dating of carbonates with the $^{230}Th/^{234}U$ method, increasing the accuracy of the method, introducing a double spike, developing various measurement protocols, widening the limits of the age range.
- Examination of the hydrogen and oxygen isotope composition of fluid inclusions of stalagmites in order to reconstruct the past cave environment.
- Climate reconstruction based on recharge temperatures and chronology of groundwater on various time scales.
- Method development for the purpose of determining the lithium isotope ratio ($\delta\,^{7}Li$) of groundwater, investigation of the lithium content of deep waters, reconstruction of the evolution of lithium.

Supervisor: **Dr. Róbert Erdélyi** **PF4/442-15**

Role of marcospicules 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. Macropsicule can be distinguished by their spatial properties and often are seen as one of two types:. They could develope 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 revail 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 roes in the heating the lower solar atmosphere. We will focus on investigatign the relation between macrospicules and TRQs in order to revail what they 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 (Sheffeild Advanced Code) and will collaborate with colleages from DHO (Debrecen Heliophysical Observatory).

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

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**

Magnetodydrodynamic 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 provied by the Solar Activity Magnetic Monitor (SAMM) 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.

Supervisor: **Dr. Mihály Molnár** **PF4/447-18**

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

Within this research, the candidate will develope procedures for sampling, sample preparation and measurement of the most modern stableisotope 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 Rind-Down Spectroscopy) will be introduced in the laboratory for the stable isotope analysis of the atmospheric methane and carbon-monoxide.

Supervisor: **Dr. Róbert Huszánk** **PF4/448-17**

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 is different applications.

Supervisor: **Dr. Gábor Battistig** **PF4/449-20**

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.

Supervisor: **Dr. Károly Tőkési** **PF4/450-20**

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

Supervisor: **Dr. Mátyás Hunyadi** **PF4/451-21**

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.

Supervisor: **Dr. Nigel John Mason** **PF4/452-22**

Space radiation - mitigation and adaptation

The next decade will see humanity retum 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 inc1ude 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 Buch as lunar and MaÍtian regoliths both as building materhds and as a source of water, oxygen, … etc, thus testing lunar and Martian regolith analogues will be important.

Sinultaneously 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 levelleading to macroscale damage. such a model is statistica1 in nature and requires inclusion of both quantum mechanical nature of atomic/molecular damage and a stochastical approach to the propagation of such damage to the macroscale. The final model shouldbe predictive in nature in order to assign risk to structural failure (and biological effects).

Supervisor: **Dr. Elemér László** **PF4/453-23**

Effect of cloud physical processes on the isotopic composition of water

The development of stratiform and convective precipitation differs significantly in space and time, owing to differences in vertical air motions and microphysical processes governing rain formation. Stratiform cloud is characterized by a large horizontal extent with weak updraft movements, while convective cloud is characterized by a large vertical extent with strong updraft movements. These different mechanisms of rain formation and cloud physics processes give the precipitation a characteristic isotope composition, which can be better understood by examining the weather parameters. The main hypothesis of the research is that the varying proportion of stratiform and convective rain types control the short-term natural variability of water isotope composition in precipitation, with other factors such as precipitation amount, temperature, and storm track having a secondary role. We propose to answer the following questions.
(1) Does the value of tritium concentration reflect the proportion of stratiform and convective precipitation in the Carpathian Basin?
(2) Is the tritium concentration in precipitation influenced by the varying frequency of mesoscale convective systems?

(3) Can the mixed precipitation – stratiform and convective together – be characterized by a specific isotope composition (3H, δ 2H, δ 18O, δ 17O)?
(4) How does the concentration of tritium in precipitation vary across different source regions with different geographical features?
(5) Do local or large-scale atmospheric processes determine the variation of tritium concentration?
(6) In addition to the tritium concentration, can 17O-excess be used as an independent hydrological tracer to determine the moisture source regions?

Supervisor: **Dr. Gábor Battistig** **PF4/454-23**

Development of printed electronics

The aim of the research is to present the application of the technological development and implementation of electronic processes and components, which are suitable for the production of flexible, even wearable, electronic units. The technology used is based on some kind of printing process and is aimed at producing conductive, dielectric and possibly sensor layers that can be implemented on a polymer substrate. The student begins his work with a thorough literature review, during which he studies the current results of materials and technologies used in printable electronics. Based on the literature, he selects the materials and technology framework in which he will carry out his experimental work. He creates test structures and test circuits that demonstrate the applicability of the developed technology. It studies and analyzes the mechanical and electrical properties of the produced test structures using material testing methods, and optimizes the technology. The field of use of printable, flexible electronics is very broad. Searches for, recommends and demonstrates various applications - e.g. chemical or biomedical sensors - areas.

Possible qualification of the applicant: degree in electrical engineering or physics or materials science, proficiency in electronics and manufacturing technology, English language skills.

Supervisor: **Dr. L. Viktor Tóth** **PF4/455-24**

Galaxies and star formation at various cosmological epochs

The largest known structures of the Universe such as the Hercules–Corona Borealis Great Wall, the Giant GRB Ring and the Huge Large Quasar Group are all inhomogeneities of special objects (gamma-ray bursts and quasars) in space time. Do these structures correspond to mass density concentrations or rather a pattern of some other peculiarity such as for example the galaxies' average star formation rate (SFR), metallicity or special galaxy interactions?

Cosmological simulations should be used to trace the large-scale structure, the mass build-up in events involving various galaxies, and the time dependent variation of galaxy parameters.
The student must develop and implement dedicated software tools. The simulations should be confronted to archival data and dedicated new measurements. These may include optical, infrared and radioastronomical observations, ground based (also interferometric) and

spaceborne. It is also necessary to examine nearby galaxies as test cases to study the processes within the galaxies with a high enough spatial resolution.
The goal is to explore the patterns in the large-scale distribution of galaxy parameters.

The research should be carried out in international collaboration with colleagues at the Ludwig Maximilian University Munich, the LAM Marseille and at the IPAC Pasadena.
Results must be presented at international conferences and published in high impact factor refereed journals.

Supervisor: **Dr. L. Viktor Tóth** **PF4/456-25**

Galactic and extragalactic star formation

Star formation alters the appearance and chemical composition of the Universe. Its raw material is cold interstellar gas. There are transport processes on various scales which feed star forming galaxies, direct the diffuse medium into interstellar filaments and star forming cores embedded into those filaments. Feed and feedback regulate the star forming rate in both galactic and extragalactic scales. The proposed research will study these processes in galactic star forming regions and in extragalaxies.
The student must use measured data describing the star formation in the 2kpc environment of the Solar System (see as Local Spiral Arm). Stability and interaction models should be tested. This experience should be used interpreting processes in other galaxies with special focus on the most active star forming regions, and the interactions of the massive stars with their environment.
There is a considerably large data base to be used, such as for example the EUCLID, Gaia, Herschel, JCMT archives. Additionally, the doctoral student should utilize the data base built by the international research team the student will be integrated into. That includes observations carried out using the Effelsberg-100m, JCMT, ALMA and other ground-based mm and sub-mm observatories. The observational data base should be enlarged if needed.
The research should be carried out in international collaboration with colleagues at the Helsinki University, IRAP Toulouse and Shanghai Astronomical Observatory.
Results must be presented at international conferences and published in high impact factor refereed journals.

Supervisor: **Dr. Péter Petrik** **PF4/457-25**

Integrating experimental and theoretical approaches for tailoring composite nanostructures

Composite nanostructures are at the forefront of energy storage, catalysis, and optoelectronics due to their unique structural and functional properties. They also enable precise control over properties such as conductivity, catalytic activity, and optical performance. However, achieving these goals requires the coupling of experimental fabrication techniques with theoretical modeling. The aim of the present research is to combine advanced experimental methods (such as combinatorial sputtering and optical metrology) with advanced computational modeling to optimize the properties of composite nanostructures for targeted applications. The combinatorial sputtering technique enables the rapid development of composite materials with diverse compositions and morphologies. On the other hand, theoretical models that are accurate predictors of nanostructure formation and electronic properties reinforce experimental methods. The integration of these methods has great potential in materials design. To understand the formation and properties of nanostructures, characterization techniques such as in situ optical spectroscopy, most importantly spectroscopic ellipsometry will be used, which allow real-time monitoring of structural changes during fabrication and annealing. Regarding morphology, composition and surface properties, surface analysis methods such as secondary electron microscopy, X-ray photoelectron spectroscopy and atomic force microscopy provide detailed insights. Theoretical modeling plays a fundamental role in predicting and optimizing the properties of composite nanostructures. The optical response of the materials will be calculated by the transfer matrix method, finite element methods, rigorous coupled wave analysis, and finite-difference time-domain approaches, as well as a range of dispersion equations. Integrating experimental data with theoretical models will accelerate the design and optimization of effective materials.

Supervisor: **Dr. László Palcsu** **PF4/458-26**

The determination of the natural level of tritium in precipitation and its link to the solar cycle

Continental ice accumulations can provide records of past climate and environmental conditions of mid- and low latitudes, complementary to polar ice cores. Observed seasonal variations in stable isotopes, dust particle concentrations, soluble ions, and black carbon have been used for ice core dating. The shallow layers are dated with the tritium distribution of the ice deposit. Since tritium is cosmogenic isotope, the influence of the solar cycle might be seen in the natural variation. Indeed, a study on an ice core retrieved in the Swiss-Italian Alps has provided an evidence that the natural variation of tritium is modulated by the solar cycle. The objectives of this research topic are structured around five topics:

1. In-depth study of tritium records of newly drilled ice cores to confirm the link between cosmogenic tritium and the 11-year solar cycle.
2. Determiantion of natural level of tritium.
3. Sr-Nd-Hf signatures of dust preserved in ice layers for provenance analysis and tracking regional/hemispheric atmospheric circulation over the ice core sites.
4. Evaluation of the plutonium isotope profiles in ice cores of remote areas (i.e. Tien Shan).

Supervisor: **Dr. L. Viktor Tóth** **PF4/459-26**

Kinematics of the Interstellar Medium in Galaxies

What shapes the morphology of galaxies? What are the driving mechanisms of star formation, and essentially the evolution of galaxies? This topic has been studied for decades using high-resolution observations and state-of-the-art models. Nevertheless — and especially thanks to JWST measurements and ongoing large-area sky surveys — the field is currently experiencing a renaissance. By observing and modeling the kinematics of the interstellar medium, we can also draw conclusions about the gravitational potential of galaxies and the physical processes operating within them. The required modeling — in the case of nearby dwarf galaxies — can be carried out with only minor further development of existing numerical tools.

The doctoral student’s main task is the analysis of high angular and spectral resolution spectroscopic observations. The data are primarily provided by radio interferometer systems, therefore prior experience in this wavelength domain is an advantage. The observations and models need to be complemented with a kinematic description of the stellar content of the galaxies. It is advisable to start the work by studying dwarf galaxies and to make use of existing large international databases as well.
The work must be carried out as a member of an international research group. The results should be presented at the research group’s meetings, at international conferences, and published in high-impact peer-reviewed journals.

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 (pT): by thermal production at low pT, quark Bremsstrahlung and jet-photon conversion at medium pT and the isospin-effect and/or modifications of the structure functions at high pT. 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. 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 antirotonic heliem 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 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 scaler 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 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-theoric 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 einvironment 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 similary 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 form 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 form 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. 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 detec-tion 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 accelaration 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) elecromagnetic 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 radiaton 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 pi0 and eta, 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 pi0 and eta, 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 pi0 and eta 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 eta, K0S and omega mesons in 200 GeV Au+Au collisions in the PHENIX experiment at RHIC

The measurement of hadrons produced at high transverse momenta (pT) is a well established tool in the study of the hot and dense medium produced in relativistic heavy ion collisions. The highest pT has been reached so far with the lightest hadron (pi0), 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 (omega) and also hadrons with hidden or open strangeness (eta and K0S). 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 eta production in the eta -> gamma gamma decay channel, omega production in the pi0 gamma, and, if feasible, production in the K0S -> pi0 pi0 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.