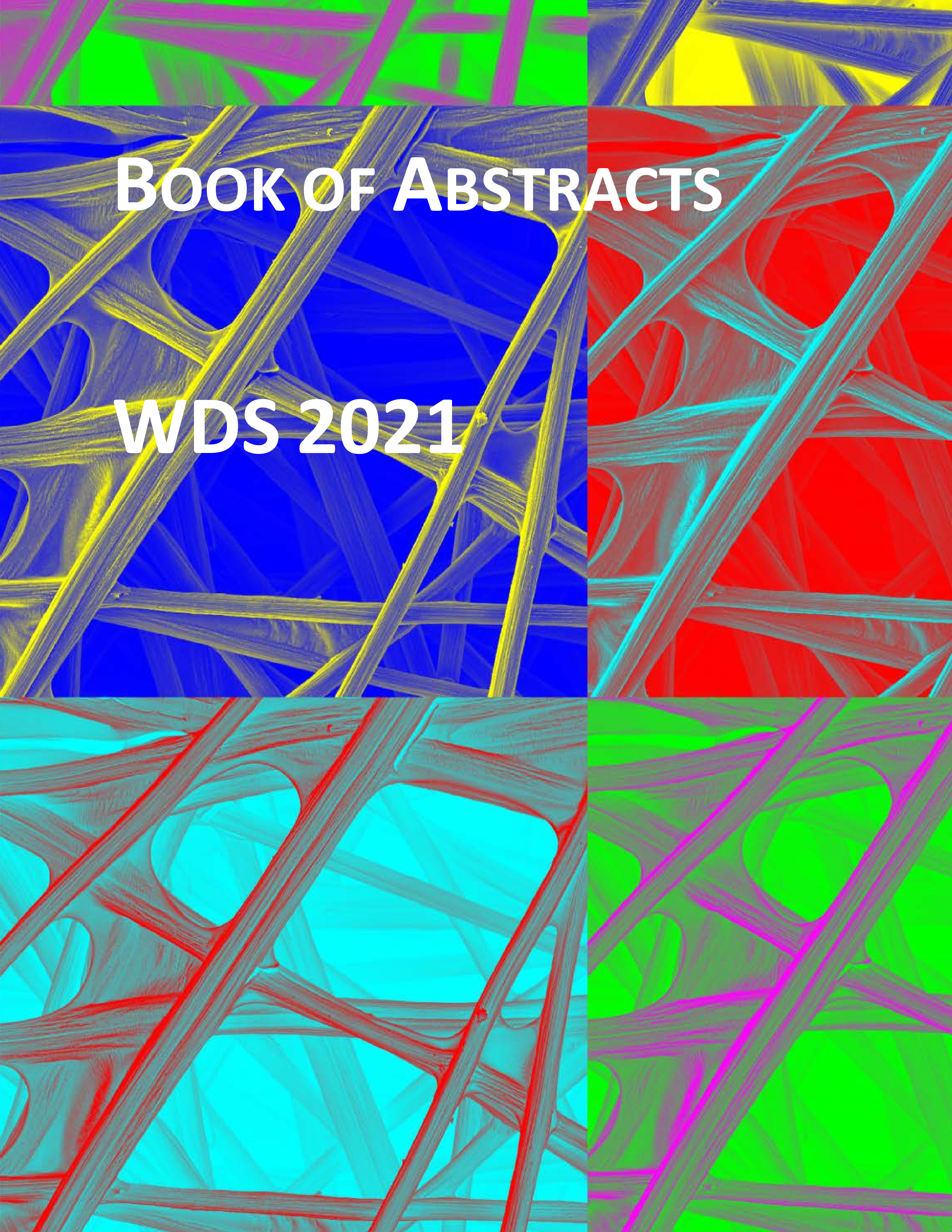
Book of Abstracts

WDS 2021



BOOK OF ABSTRACTS

Week of Doctoral Students 2021

Prague, June 15–17, 2021

CONTENTS

Abstracts are listed alphabetically
by presenting authors in each section.

F-1 Theoretical Physics, Astronomy and Astrophysics

On the Light Rays Propagating in Plasma Medium around Relativistic Objects

Bezděková B.*, *Balek V.*, *Bičák J.

Abstract. When emitted from distant galaxies, light rays may propagate through regions with matter (especially plasma), not only through vacuum. A precise specification of the medium is important — it can cause the rays to change substantially their form. If the rays are passing near a strongly gravitating compact object, both plasma and gravitational effects have to be taken into account. The impact of refractive and dispersive media around compact objects is typically relevant in problems related to the gravitational lensing. In our work we focus on how the regions allowed for propagation of rays in the equatorial plane of a rotating black hole are modified due to the presence of the refractive and dispersive media with various density profiles. We investigate the media with the density distributions corresponding to typical profiles of lensing galaxies, as well as with the density distribution of a nonsingular isothermal sphere. We show that the regions permitted for the rays in a medium are substantially reduced as compared with the corresponding regions in vacuum. We also study allowed regions as seen by observers freely falling onto the black hole from the rest at infinity.

Geodesic Chaos Around Perturbed Black Holes

Caputo C.*, *Semerák O.

Abstract. Geodesic motion is completely integrable in the fields of isolated stationary black holes, but it may become chaotic if there exists some additional source in the space–time. The aim of the talk is to review previous results, in which the dynamics of such a system has been investigated by restricting to the static and axisymmetric case, and to outline future plans in which the research will be extended to the stationary case in order to study how the rotational dragging affects the chaoticity of the dynamics.

Vertex Operators in Ambitwistor Strings

Carabine N.

Abstract. I will give a brief introduction to string theory and Ambitwistor Strings. Following this I will discuss the Ambitwistor string's main features, issues and recent developments. In particular I will show that the physical spectrum describes higher derivative field theories.

OGLE-BLG504.12.201843: An Extreme Dwarf Nova

Landri C.

Abstract. Dwarf novae (DN) are binary star systems composed of a white dwarf accreting from a companion star. DN undergo periodic brightening caused by instabilities in the accretion disc. I present new spectroscopic data and analysis of archival photometry for OGLE-BLG504.12.201843. This object displays periodic large outbursts that last for hundreds of days and short flares that appear during the quiescence state. Together with spectroscopy, this evidence suggests that this object is a DN with extreme properties.

Minimal Mass Ratio of Contact Binaries

Pešta M.

Abstract. When two low-mass stars in a close orbit evolve, they expand, get into contact, and start sharing a common envelope. Such a system then gradually evolves to smaller mass ratios until a critical value is reached, at which moment it undergoes the Darwin instability, leading to a rapid merger and observable brightening. In this talk, I will present a preliminary estimate of this critical threshold obtained with the help of newly available space-based data and ground-based spectroscopic surveys.

X-ray Polarization of Black-hole Accretion Discs in Active Galactic Nuclei

***Podgorný J.**, Dovčiak M., Marin F., Matt G., Goosmann R., Różańska A.*

Abstract. We present the theoretical spectrum and polarization properties of X-ray emission from accretion discs in active galactic nuclei (AGN). The reflected radiation from an accretion disc illuminated by a corona above is computed using the Monte Carlo radiative transfer code STOKES. The structure of the disc, modelled as a constant density slab, has been computed with the TITAN code for optically thick and hot photo-ionized media. Further, we use the relativistic code KYNSTOKES based on our well-tested relativistic KY package to account for all relativistic effects on radiation near a black hole and to compute the total disc emission as would be detected by a distant observer. It is then possible to predict X-ray spectral and polarization properties of an accretion disc in AGN and their dependence on various parameters of the system (spin of the black hole, ionization of the accretion disc, observer inclination). This is fundamental for the interpretation of AGN spectra and polarization obtained by the IXPE mission or the eXTP mission.

Optically Dark Clouds in the Cluster of Galaxies

***Sabzali V.**, Wunsch R.,*

Abstract. 21cm surveys of the Virgo cluster of galaxies discovered optically dark clouds with velocity dispersions >100 km/s. This suggests dynamical masses ≈ 10^{10} M_{Sun}, while their line brightness masses are ≈ 10^{7} M_{Sun}. They are not angularly resolved implying sizes < 17 kpc. We hypothesize that they are dark galaxies, i.e., dark matter halos with not enough baryons to form stars. We plan to test it by simulations using the code Trixi. We will analyze our VLA observations and compare them to the simulations.

Composition of Cometary Dust from Fireball Spectroscopy

Šegon M.

Abstract. The study is part of the grant project Compositional and orbital mapping of meteoroid sources in the Solar System. It focuses on the analysis of analog and digital spectra of fireballs and aims to improve our knowledge of the composition of cometary meteoroids. Comets and meteors are defined, followed by a basic introduction to meteor spectra and the current knowledge of the field. The equipment and spectral analysis approach are described, concluding with a current progress report and plans.

Consequences of Gravitational Wave Observations on Dark Energy

Creminelli P., Tambalo G., Vernizzi F., Yingcharoenrat V., Sawicki I., Trenkler G.

Abstract. I will discuss some of the implications of recent gravitational wave observations on (single field) dark energy/modified gravity models belonging to the class of Scalar-Tensor theories. More specifically, I want to comment on the claim made in the literature that a subclass of these theories (which do not modify the speed of tensor perturbations) feature an instability in the cosmological background in the presence of strong gravitational waves, rendering such modifications of gravity unviable.

A Review of Spherically Symmetric Solutions in Quadratic Gravity

Turner G.

Abstract. Recent study of the spherically symmetric vacuum solutions to the field equations of quadratic gravity, using both analytical and numerical techniques, indicates the existence of a wide variety of spacetimes not present in standard general relativity. This presentation will summarize the techniques employed to investigate these spacetimes and highlight some interesting cases. GR spacetimes will be identified as limits of the more general QG ones and future research will be outlined.

Evolution of Accretion States in Stellar-mass Black Hole X-ray Binaries

Yilmaz A., Svoboda J.

Abstract. X-ray spectral studies of stellar-mass black hole X-ray binaries (BHXRBs) showed that these systems follow an evolutionary path going through different accretion states. We aim to perform a systematic investigation of this evolution in BHXRBs by studying the relativistic effects on the accretion disk emission. We intend to enhance previous works by increasing the quality of statistical representation of the thermal X-ray emission from the disk by using a wider range of instruments with higher sensitivities.

F-2 PHYSICS OF PLASMA AND IONIZED MEDIA

Small-scale Kazantsev Dynamo-model in the Frame of Turbulent Cascade Approach

Abushzade I.*, *Yushkov E.

Abstract. Traditionally the dynamo theory describes the large-scale magnetic field generation in the turbulent plasma systems, for example, in the convective stellar shells or galaxy disks. But, the dynamo equations, obtained by averaging of the magnetic induction low over a random velocity field also describe the small-scale, so called turbulent, dynamo, a characteristic feature of which is magnetic energy growth with zero first moment. The first linear small-scale dynamo model was suggested by Kazantsev for short-correlated in time turbulence. In this report we speculate about the cascade model, which is obtained by Fourier transformation of mhd-system on a spectral shell. This model is generally nonlinear and its nonlinearity provides the mutual exchange of magnetic/hydrodynamic energy and helicity between the shells. We compare the numerical results of Kazantsev model and the cascade one, highlight the linear and nonlinear dynamo regimes, show the dependence of dynamo-generation on the hydrodynamical properties of the turbulence. Basing on the obtained results, we discuss a possible role of small-scale generation in the large-scale dynamo by reverse helicity transport along the specter.

Mean Field Dynamo-model in Locally Anisotropic Inhomogeneous Turbulent Flow

Allahverdiyev R. R., Yushkov E. V., Sokoloff D. D.

Abstract. The averaging of the magnetic induction equation over a random velocity field forms the basis of the dynamo theory, which describes the formation and evolution of large-scale astrophysical magnetic fields. The standard approach is the asymptotic method, proposed by Krause and Radler in the 1960's for two-scale plasma turbulence. Two-scale assumption assumes that a random velocity field can be represented as a sum of a large-scale slowly varying component and a small-scale fluctuating one. Exactly by this method the classical systems of the Parker Solar dynamo and the galactic disk dynamo were obtained. In our report we discuss a different method of the averaging, proposed in 1985 by Molchanov, Ruzmaikin, and Sokoloff for working with a short-correlated in time random flow. It does not require the assumption of a spatial two-scale velocity field structure and easily allows one to derive the dynamo equations for both the first and the second magnetic field moments in locally anisotropic and inhomogeneous conditions. The advantages of the functional integral approach and possible areas of its application in astrophysical plasma are discussed.

Design of COMPASS-U Support Structure Cooling

Barton P., Zelda J., Sestak D., Zhang H., Ficker O., Varju J., Havlicek J.

Abstract. COMPASS-U will be new tokamak, currently in construction at IPP Prague. Its main design features include copper coils, cryogenically cooled to reach required toroidal field of 5 tesla. All the coils are held in place by massive stainless-steel support structure, designed to significantly limit coil movement. To cope with thermal shrinkage of coils, support structure will be also cooled by gaseous helium cooling system, whose analysis, design and engineering is described on this poster.

Study of Alpha Particle Properties Across Rarefaction Regions

Ďurovcová T., Šafránková J., Němeček Z.

Abstract. When the fast stream outruns the slow stream, a corotating rarefaction region (CRR) is formed. CRRs are characterized by a monotonic decrease of the solar wind speed, and they are associated with the regions of small longitudinal extent on the Sun. In our study, we use near-Earth measurements complemented by observations at different heliocentric distances, and focus on the behavior of alpha particles in the CRRs. We apply a superposed-epoch analysis of identified CRRs with a motivation to determine the global profile of alpha particle parameters through these regions. Next, we concentrate on the cases with largest A_{He} variations and investigate whether they can be associated with the changes of the solar wind source region or whether there is a relation between the A_{He} variations and the non-thermal features in the proton velocity distribution functions like the temperature anisotropy and/or presence of the proton beam.

Whistler Wave Instability in Multi-component Electron Plasma of the Earth's Magnetosphere

Frantsuzov V. A., Shustov P. I., Artemyev A. V.

Abstract. Whistler-mode waves play a crucial role in electron acceleration and scattering in the Earth's inner magnetosphere. The main energy source of this wave mode is the free energy of the thermal anisotropic electron populations injected into the inner magnetosphere from the magnetotail. The theoretical model for the wave generation threshold has been constructed only for a one-component anisotropic plasma. However, spacecraft observations show that intense whistler-mode waves often observed in the multicomponent plasma, where the threshold for wave generation is unknown. This work aims to generalize the existing theory of whistler-mode wave generation to more realistic multi-component plasma. Thermal anisotropy of such systems can be significant, but well localized within a narrow. Thus, whistler-mode wave instability can be observed even with a low level of the averaged anisotropy. To describe this effect, we have derived the instability threshold for multicomponent plasma and investigate how parameters of different plasma populations affect the whistler-mode wave generation.

Kinetic Monte Carlo Simulations of Polaronic Diffusion in Titanium Doped Hematite

***Gabriel V.**, Kocán P., Setvín M., Redondo J.*

Abstract. Hematite is a promising material for photoelectrochemical water splitting. A key impediment for applications is the slow kinetics of charge transfer caused by the formation of small polarons. It has been experimentally observed that titanium doping enhances the polaron migration, but without a sufficient theoretical model. Here we present a kinetic Monte Carlo model of polaron diffusion, where the influence of dopants is modeled by several different approaches and compared to experimental data.

Variations of Energetic Particle Fluxes Around Significant Geomagnetic Storms Observed by the Low-altitude DEMETER Spacecraft

***Gohl S.**, Nemec F.*

Abstract. A superposed epoch analysis is conducted for five geomagnetic storms in the years 2005 and 2006 with the aim to understand energetic particle flux variations as a function of L-shell, energy, and time from the Dst minimum. Data measured by the low-altitude DEMETER spacecraft are used for this purpose. The storms are identified by a Dst index below –100 nT, as well as being isolated events in a seven-day time window. We show that they can be categorized into two types. The first type shows significant variations in the energetic particle fluxes around the Dst minimum and increased fluxes at high energies (>1.5 MeV), while the second type only shows increased fluxes around the Dst minimum without the increased fluxes at high energies. The first type of storms is related to more drastic but shorter-lasting changes in the solar wind parameters than the second type. One storm does not fit in either category, exhibiting features from both storm types. Additionally, we investigate whether the impenetrable barrier for ultra-relativistic electrons holds also in extreme geomagnetic conditions. For the highest analyzed energies, the obtained barrier L-shells do not go below 2.6.

Detection of Dust Grains by MAVEN Using Electric Field Instruments

***Ijaz S.*, Vaverka J.**

Abstract. Detection of dust grains in space is limited by a small number of dedicated dust detectors, however we aim to study dust detection by using electric field instruments usually placed on the majority of scientific spacecraft. The major advantage of this technique is that entire spacecraft surface acts as a detector. The main objective of this work is to study pulses generated by dust impacts on the Mars Atmosphere and Volatile Evolution (MAVEN) spacecraft. We show some preliminary results onto the spacecraft body during the event.

Characterisation of Sawtooth Instability at COMPASS

***Imrisek M.*, Weinzettl V, Jaulmes F., Bogár K., Seidl J., Tomes M., Bílková P., Hron M.**

Abstract. At COMPASS, sawtooth instability is shown to have significant effect on various plasma processes such as occurrence of edge localized modes (ELM) or transitions to H-mode, ELM-free H-mode or L-mode. The contribution also deals with the effect of main plasma parameters on sawtooth period, its inversion radius and kink mode preceding sawtooth crash.

On Slow Electron Holes in the Earth's Magnetosphere

Kamaletdinov S., Vasko I., Artemyev A.

Abstract. Electron holes are a solitary wave of BGK type. Interest in such structures is due to the fact, that they may contribute to plasma heating and provide anomalous resistivity in various space plasma regions. Multisatellite space observations of electron holes have firmly established that these structures can have speeds comparable to ion thermal velocity. This fact presents a sort of an obstacle since the established theory of electron holes based on the assumption that ions are not perturbated. In our work we elaborate a model that adjusts the classical one by taking ion response into account. Based on measurements aboard MMS spacecraft, we found a homogeneous cluster of electron holes in the Earth's plasma sheet. We show that background ion VDFs have a pronounced double-humped shape with electron hole speeds clustered near the local minimum. We elaborate a way to integrate the ion response into the BGK procedure thus obtaining a model that comprehensively takes ion response into account. In the frame of this model, we obtain new parametric regions available for the structures and estimate the trapped electron population. The problems of stability and acceleration are discussed.

Diagnostics of Reactive HiPIMS Discharge Assisted by ECWR Plasma

Kapran A., Hubička Z., Tichý M.

Abstract. This study focused on the investigation of plasma parameters in reactive HiPIMS for two different configurations — conventional HiPIMS and hybrid system HiPIMS assisted with the electron cyclotron wave resonance (ECWR) discharge. In r-HiPIMS+ECWR configuration a discharge could be maintained at working gas pressure lower than typical for conventional r-HiPIMS. Due to reduced pressure the plasma parameters such as electron temperature and ion flux density differ from common HiPIMS. The measurements were performed using an iron target in Ar/O_2 atmosphere. Plasma parameters have been studied as a function of varying oxygen flow rate during magnetron sputtering process. The diagnostics of plasma was performed by means of RF planar ion flux probe at the position of the substrate.

Properties of Electromagnetic Signals Generated During the Development of Natural Lightning Discharges

Kolinska A.*, *Kolmasova I., Santolik O., Defer E., and Pedeboy S.

Abstract. Analysis of electromagnetic signals emitted by natural lightning discharges is a way to investigate all evolution stages of lightning flashes. Lightning initiation and development of activity following the first return strokes for selected cloud-to-ground flashes from the data collected in the Mediterranean during autumn 2015 are presented. Measurements of the broadband receiver BLESKA are compared to the sources of narrowband VHF radiation detected by Lightning Mapping Array SAETTA.

Magnetic Field Coils Misalignments on the COMPASS-U Tokamak

Kripner L.*, *Krbec J., Háček P., Markovič T., Ficker O., COMPASS team

Abstract. The toroidal asymmetry of the tokamak magnetic field can lead to unwanted MHD instabilities and decrease plasma confinement. The asymmetry is introduced to the system by the realistic coil winding and possible manufacturing misalignments. In this contribution, the effects of toroidal and poloidal magnetic coils misalignments with realistic winding are analyzed using Monte Carlo calculations. From effects are evaluated by calculations of error field coefficient and by use of Fourier analysis.

Kinetic of Ion Molecular Interaction Simulator

Lacko M.*, *Spanel P.

Abstract. Kinetics of Ion Molecular Interaction simulator (KIMI) is a Windows based application build to assist the chemical ionization analytical instruments. The proposed set of ion molecular reactions is interactively drawn in a graphical interface and converted into a set of differential kinetic equations. The simulator numerically solve sets of kinetic equations describing changes of reagent and product ion number densities along the axis of the reactor and thus model ion intensities presented within and at the end of the reactor tube.

Lumped Circuit Model for Eddy Currents in Tokamak Passive Structures

***Markovic T.**, Kindl V., Duran I., Turjanica P., Balner V., Weinzettl V.*

Abstract. Passive conducting structures of a tokamak (e.g. vacuum vessel or stabilizing plates) are inductively coupled to the toroidal current of the confined plasma. As a result, changes in plasma position or plasma current induce eddy currents in these structures that affect the magnetic sensor signals and need to be accounted for. A lumped circuit model of passive structure eddy currents developed for tokamaks COMPASS and COMPASS-U, validated by Ansys Maxwell software, is presented in this work.

Current Flows Towards the Divertor During VDEs at COMPASS

***Matveeva E.**, Artola F.J., Havlicek J., Lehnen M., Pitts R., Roccella R., Adamek J., Cavalier J., Dejarnac R., Jerab M., Sestak D., Barton P.*

Abstract. Unmitigated disruptions pose an important issue for future fusion devices as they might prevent sustainable operation of tokamaks. Solid physics basis is needed for estimation of mechanical loads on the vacuum vessel. Determination of vessel currents magnitude and their path play a key role in understanding of electromagnetic loads. This work aims on testing the model of asymmetric toroidal eddy currents (ATEC) using special divertor tiles installed at the COMPASS tokamak. It shows that alternative vessel currents paths through the plasma facing components is possible.

Analytical Evaluation of Plasma Parameters by Optical Emission Spectroscopy in Low-Pressure Hollow Cathode Plasma Jet and Planar Magnetron System by DC and Pulsed DC Excitation Source

Mishra H., Kudrna P., Tichy M.

Abstract. Optical emission spectroscopy (OES) unified with the models of plasma light emission becomes a non-intrusive and versatile method for plasma parameters determination. Each spectral line in emission spectroscopy corresponds to an optical transition between two quantum levels of atom/molecule. The number density of gas species in the upper state determines the spectral line intensity. The spectral line intensities regulate densities of species in various states by some population models. With the utilization of various population models, one can calculate the dependence of different spectral line intensity ratios versus various plasma parameters. The analytical evaluation of plasma parameters in the low-pressure regime for hollow cathode plasma jet and planar magnetron system in presence of DC and pulsed-DC excitation source were performed successfully. The effect of various processing parameters like power, working pressure, flow rate, and frequency (constant duty cycle) on plasma parameters had been investigated in presence of argon gas atmosphere.
Keywords; Optical emission spectroscopy, Low pressure, Hollow cathode plasma jet, Planar magnetron, DC, Pulsed DC

Ion Trap Study of the Isotope Exchange Reaction of OH^- with HD

Palacký J., Rednyk S., Roučka Š.

Abstract. The isotope exchange reaction $OH^- + HD \Rightarrow OD^- + H_2$ was studied at astrophysically relevant temperatures. We used a 22-pole cryogenic ion trap that allows us to measure in the temperature range from 300 K down to 10 K.

Understanding the Plasma Rotation in the COMPASS Tokamak

Peterka M., Seidl J., Casolari A., Jaulmes F., Tomes M., Zadvitskiy G., Bogar K.

Abstract. Plasma rotation is an important phenomenon in tokamaks as it improves the confinement and stability, it is also an essential parameter for kinetic plasma modeling, but there is no measurement routinely available in the COMPASS tokamak. In this work, the relation between the MHD fluid velocity, the rotation of impurity ions, and the frequency of magnetic fluctuations due to the rotation of magnetic islands is evaluated using the neoclassical theory and compared with experimental observation.

Low-frequency Fluctuations in the Foreshock: Effect of the Lunar Wake

***Salohub A.**, Šafránková J., Němeček Z.*

Abstract. Low-frequency (ULF) waves fill most of the upstream region that is connected to the bow shock by the interplanetary magnetic field (IMF) lines. The foreshock waves are generated by ion beam instability excited by counter-streaming flows of the incident and reflected ions. However, the Moon coupled to its wake is a large obstacle that can affect the trajectory of energetic particles. Our previous global statistical study over nine years shows that waves could be growing as well as decaying towards the bow shock under the quasi-radial magnetic field. In this work, we investigate the influence of the lunar wake on the activity of ULF waves in the Earth's foreshock for the same IMF condition. We chose a statistical approach to compare two sets of data (global and effect of the lunar wake) with motivation to estimate factors influencing the growth rate of ULF fluctuations near the Moon and lunar wake. We study the conditions for growing and damped fluctuations under different solar wind parameters. With this information, we discuss the role and importance of the different trajectories of wave propagation through the lunar wake and possible mechanisms that can lead to the observed results.

Recombination of H_3^+ Ions with Electrons in Ambient Neon Gas

***Shapko D.**, Dohnal P., Roučka Š., Uvarova L., Kassayová M., Plašil R., Glosík J.*

Abstract. A Cryogenic Stationary Afterglow experimental setup equipped with continuous wave Cavity Ring-Down absorption Spectrometer (Cryo-SA-CRDS) for precise measurement of ion number densities decay in afterglow plasmas was modified by adding time resolved microwave diagnostics for direct determination of electron number density in the temperature range of 30–300 K. The new abilities of our apparatus were demonstrated on measurements of H3+ recombination in neon buffered plasmas at conditions where H3+ ions are not dominant ions in the afterglow.

Raysect and Cherab Framework for Forward Modelling of Optical Plasma Diagnostics

Tomes M.*, *Lovell J., Neverov V. S., Carr M., Meakins M., Giroud C., Sos M.

Abstract. Raysect and Cherab is a framework for modelling of plasma optical diagnostics. Raysect is a general-purpose 3D ray tracing engine and Cherab is a library of plasma radiation models. The framework allows characterization of optical plasma diagnostics and can aid their design or enhance determination of plasma properties from measured data. The aim of this talk is to introduce the framework to the audience and to give a broad overview of its capabilities and applications.

Dye-sensitized Solar Cells Based on Iron Oxide and Sulfide Films

Tuharin K.*, *Kudrna P., Tichy M.

Abstract. The perspectives of iron oxide films and it sulfidation for dye-sensitized solar cell (DSSC) will be reviewed. The hollow cathode plasma jet (HCPJ) sputtering technique at both DC and high-power DC pulsed regimes will be described with respect to iron oxide film deposition. Plasma composition was measured by mass spectrometer. AFM, SEM, EDX and Raman spectroscopy of films are presented. Keywords: hollow cathode plasma jet, iron oxide, iron sulfide, dye-sensitized solar cell

Facilitation of the Underwater Discharge Initiation with the Use of a Marx Generator

Tuholukov A.*, *Stelmashuk V.

Abstract. The process of underwater discharge formation consists of three successive stages: an initiation phase, a streamer propagation phase and a spark phase. For the number of technical applications different methods of facilitation of streamer propagation are necessary. This work presents investigation of the method of discharge initiation by preliminary high-voltage spark produced by Marx generator

Study of Nanoparticles in the Hollow Cathode System with Laser Beam Scattering

Turek Z., Kudrna P.

Abstract. According to previous research, the hollow cathode deposition system can be source of nanoparticles. The research was done by laser beam scattering with measurement of intensities in three directions. The goal of this study is to enhance the experimental setup to be able to measure scattered light intensity in all directions. Those data will be used to calculate nanoparticle's size using Mie scattering model.

Study of Rotational Populations of OH^- Anions in 22-pole Radiofrequency Ion Trap in the Temperature Range of 50–200 K

Uvarova L., Rednyk S., Plašil R., Roučka Š., Dohnal P., Glosík J.

Abstract. Abstract. Ion trap technique in combination with photodetachment spectroscopy was used to study the thermalization of OH^- in the temperature range of 50–200 K. The ions were trapped in a multipole radiofrequency trap and cooled by helium buffer gas. The photodetachment spectra were recorded as a dependence of OH^- losses in trap on frequency. The preliminary results show an excellent agreement between the OH^- rotational temperature and the temperature of 22-pole trap in the studied temperature range.

F-3 PHYSICS OF CONDENSED MATTER AND MATERIAL RESEARCH

Pressure-driven Structural and Magnetic Transformations in 221 Intermetallics

***Král P.*, Prchal J., Kaštil J., Klicpera M., Diviš M.**

Abstract. Family of R2T2X intermetallics crystallizing in tetragonal layered structure represent systems with potential for specific electronic properties and exhibit variety of interesting phenomena. Anisotropic crystal lattice and potential for the geometrical frustration arising from the triangular arrangement of R-atoms exhibit playground for tuning of the magnetic interactions responsible for electronic behavior by external mechanical pressure as the pure way to affect the crystal lattice without changes in chemical composition.

A Study of Modern Al–Li Based Alloys

***Kralik R.*, Krivska B., Belejova S., Bajtosova L.**

Abstract. Al–Li alloys offer low density and good mechanical properties, both of which originate from the addition of Li as the lightest metal, which can also form coherent metastable strengthening precipitates. Negative properties have also been identified such as anisotropy of properties and low fracture toughness associated with the metastable Al–Li phase, presence of coarse intermetallics and precipitate-free zones. Modern Al–Li alloys seek to limit precipitation of this phase through lower Li contents, proper processing, and precipitation of ternary Al–Li–X phases.

Growth Kinetics of Intermetallic Compounds in Al–Steel Clad Sheet

***Křivská B.*, Šlapáková M., Králík R., Fekete K., Grydin O., Stolbchenko M., Schaper M.**

Abstract. The formation and the kinetics of the growth of intermetallic layers between austenitic steel and technically pure aluminum were investigated via SEM analysis of bulk samples after annealing and TEM in-situ annealing. After the first nucleation stage, the total thickness of the intermetallic layer was governed mainly by the parabolic diffusion-controlled growth of the Al_5Fe_2 phase.

Comparison of GW Variants for Sodium Nanoclusters

***Marek Š.*, Korytár R.**

Abstract. GW approximation is a well-known approximation for calculating exchange and correlation energies of molecular systems. However, the calculation is relatively computationally demanding, restricting the pure GW to small systems. Further approximations can be made to alleviate the computational price, especially the memory requirements. The basis and implications of these approximations are discussed in the context of the calculation of energetic spectrum of sodium nanoclusters. Stability and precision of different GW variants is discussed on several model calculations.

Anisotropic Magnetoresistance in Systems with Non-collinear Magnetic Order

Ritzinger, P.

Abstract. Since its discovery in 1857, the anisotropic magnetoresistance (AMR) has been in focus of many theoretical studies. They range from rather simple s-d models to quite complex ab initio calculations. Most attention has been paid to ferromagnets and recently, the scope of research on AMR is extended to include also antiferromagnets (AFMs). The interest in AFMs is mainly motivated by the fact that magnetic order can be manipulated without having a net magnetic moment and thus AFMs are excellent candidates for future spintronic devices. The main focus of our work will be the investigation of intrinsic AMR, which is due to an anisotropic Fermi surface. This is achieved by considering non-collinear magnetic order on a Kagome lattice. Magnetic moments can be arranged in many different ways on such a lattice and seemingly small changes alter the Fermi surface and transport properties. We are investigating the influence of magnetic ordering on these properties which allows to predict general features of spin texture and transport by only considering the symmetry of the underlying system. Exemplary systems are discussed in this context.

Crystallographic and Electronic Properties of Rare-earth A2B2O7 Oxides Under Extreme Conditions

Staško D.

Abstract. Cubic rare-earth $A_2B_2O_7$ oxides, with A standing for a rare-earth element and B for a transition metal or main block element, have been systematically studied for their frequently exotic properties. In this work, we focus on the application of high pressure to tune the electronic and magnetic properties tied with the geometric frustration present within the cubic pyrochlore structure, and to study the stability of the pyrochlore and defect fluorite structures. With this goal in mind, we focus mainly on iridate ($A_2Ir_2O_7$) and zirconate ($A_2Zr_2O_7$) oxides.

F-4 Biophysics, Chemical and Macromolecular Physics

Committee Neural Network Potentials in Molecular Dynamics

Beck H.

Abstract. Machine learning promises to decrease the cost of ab initio level molecular dynamics, a tool widely used across many disciplines in chemistry and physics, by multiple orders of magnitude. Among the many different approaches, committee neural network potentials show great promise, as the committee disagreement can be used create comparatively small but efficient training sets and offers a convenient way to judge the capacity of a model with respect to a specific system.

Projection-based Embedding of DMRG Method in DFT

Beran P., Veis L.

Abstract. The Density Matrix Renormalization Group (DMRG) method established itself as one of the benchmark methods for strongly correlated systems. However, the size of the systems available for investigation is limited by ever increasing computational price. Here we present the theory and first results of our work towards alleviating this problem by combining DMRG with computationally less expensive DFT using recently developed projection-based embedding theory.

Effect of Intense Short Electric Pulses on Protein Nanostructures

Blanco Campoy D. G., Zakar T., Cifra M.

Abstract. Proteins are one of the most abundant biomolecular components of biological systems. Therefore, anomalies in proteins can give rise to diseases and serious metabolic dysfunctions. In recent years, numerous reports have indicated that applying electric fields on proteins lead to several responses. Since proteins carry electric charge, they can be affected by intense electric fields. In this research we study effects of intense short electric pulses on tubulin and related proteins using variety of spectroscopic and microscopy tools and methods. A controlled modification of protein function could open the door of a new World of possibilities for novel and advanced therapeutical methods in biomedicine and manipulation methods for bionanotechnology.

Microcrystalline Inclusions of Biogenic Guanine in Algae: Presence, Properties and Functions

Bokov M., Mojzeš P.

Abstract. Crystalline inclusions composed of guanine and related purines were identified in different photosynthetic eukaryotes. They were shown to serve as long-term, high capacity stores of nitrogen, however, they may have also other functions, e.g., light manipulation. By means of Raman microscopy, we will investigate their biosynthesis, direct uptake, and post-uptake fate. Furthermore, other possible roles of purine crystals will be studied, especially those connected with their optical properties.

Radically Different Behavior of the Solvated Benzene Radical Anion

Březina K.

Abstract. The benzene radical anion, an important organic reaction intermediate, behaves as a short-lived scattering resonance in the gas phase, but exhibits long-term stability in various polar solvents. In this work, we elucidate the stability induced by liquid ammonia using an accurate computational approach and conclusively demonstrate that the species becomes a bound state after solvation. Moreover, we investigate its highly non-trivial molecular structure governed by the dynamic Jahn–Teller effect.

Estimating the Quantum Yield of Singlet Fission Process

Fatková K.

Abstract. The aim is to improve the efficiency of solar cells above the Shockley–Queisser limit by carrier multiplication, which can be achieved via the singlet fission process. Our work aims to develop a reliable procedure which would be able to estimate the rate constants of competing processes. Using previously established method which calculates the singlet fission rate constant, it would be possible to search for the molecular packings that maximizes the quantum yield of the singlet fission process.

Luminescence Properties of Water-soluble Europium Complex at Different pH?

Charyshnikova Z.

Abstract. Changes in external conditions can have a significant impact on the luminescent properties of rare earth element complexes. The study of their luminescent characteristics at different pH values is a relevant task for the use of such compounds in medicine and biophysics. We researched the spectral-luminescent characteristics of the water-soluble europium complex in a wide range of pH. We got the dependence of emission spectra, luminescence quantum yield, lifetime, asymmetry coefficient on pH.

Membrane Asymmetry and Nanodomain Coupling

Chmelova B., Davidovic D., Šachl R.

Abstract. The cellular membrane is a complex structure playing an important role in a large number of processes. It consists of two layers that are highly asymmetric in composition and function. Heterogeneities (nanodomains) develop in lipid membranes and their distribution is the subject of our research. This work focuses on the investigation of coupling between nanodomains found in the upper and lower leaflet of the lipid bilayer. There are diverse situations based on forces formed in between the nanodomains. The forces are either attractive, repulsive or too weak to influence their mutual positions. We used MC simulations to study the resolution of MC-FRET towards inter-leaflet coupling. Its sensitivity depends on several parameters as the affinity of fluorescent probes towards the nanodomains or the bilayer thickness. We varied these parameters computationally and found out that the method is the most sensitive when donors and acceptors have either high or low affinity to nanodomains, however it can be quite complicated to find probes fulfilling those conditions. For probes with more homogenous distribution the case of donors and acceptors in different layers provides better results.

Dual-responsive Polymer Hydrogels with Double-network Structure

Hanyková L., Krakovský I., Ivaniuzhenkov V.

Abstract. The so-called smart hydrogels which are capable of responding to the changes in temperature, pH, humidity, light, specific ions or molecules, electrical fields, solvent and ionic strength, have attracted much attention because they can serve as functional materials with potential applications in the areas of drug delivery, microlenses, sensors and artificial organ. In the current project, hydrogels possessing multi-response properties depending on temperature, solvent composition and ion concentration are studied. Double network (DN) hydrogels composed of poly(N,N-diethylacrylamide) (PDEAAm), polyacrylamide (PAAm) and poly(acryl-2-amido-2-methylpropanesulfonic acid) (PAMPS) were synthesized and characterized by NMR spectroscopy and swelling experiments. The influence of DN composition on the phase transition was examined.

Superradiance in Bacteriochlorophyll c Aggregates

Malina T., Koehorst R., Bína D., Pšenčík J, van Amerongen H.

Abstract. Chlorosomes are light-harvesting antennas of green photosynthetic bacteria. Unlike other antennas, they contain almost no protein and the light harvesting is mediated mainly by aggregates of pigments, bacteriochlorophylls (BChls). Important part of their function is a highly efficient transport of the absorbed energy for processing in reaction centres. We have observed superradiance (i.e., collective spontaneous emission) in these antennas as well as in artificial aggregates of BChls. This means that fluorescence occurs from a state that is delocalized over several molecules in the aggregate and has a higher transition dipole strength than the radiative state in monomeric BChl (2-3-fold higher). The increased dipole strength increases probability of both energy transfer and radiative transition; however, the quantum yield of the aggregated BChls is decreased by several orders of magnitude (2-2.6 orders in comparison to monomeric BChl) which greatly reduces the probability of a radiative decay. Both those factors (increased dipole strength and decreased quantum yield) contribute to the high energy transfer efficiency of chlorosomes, which can be mimicked in organic photovoltaics.

Applications of the Density Matrix Renormalization Group Method

***Matoušek M.*, Veis L.**

Abstract. We present the Density Matrix Renormalization Group (DMRG) method as it is used in quantum chemistry. We show several applications of this method to challenging strongly correlated problems (Fe(II)-porphyrins, FeS clusters). Finally, we show how we plan to further extend this method, into the realm of non-Born–Oppenheimer quantum chemistry.

Metallization of Polypyrrole-coated Textiles

***Pandey A.*, Bober P., Pfleger J.**

Abstract. We developed a method of preparation of silver (Ag) coated textile based on electroplating of cotton/PES chemically precoated by a conducting polymer. By a combination of properly selected surfactant, ultrasonication, and using AgNO3, a polypyrrole precoated textile with a homogeneous Ag coating, increased electrical conductivity and mechanical stability have been obtained compared to conventional techniques. It is applicable for EMI shielding, sensors, or as a wearable electrical heater.

Rewritable Memory Device in Poly[N-(3-(9H-carbazole-9-yl)propyl)methacrylamide] with Pendant Carbazole Groups

***Panthi Y. R.*, Pfleger J., Výprachtický D., Rais D., Thottapali M. A., Pandey A., Foulger S. H.**

Abstract. We report on synthesis of poly[N-(3-(9H-carbazole-9-yl)propyl)methacrylamide] and its photophysical and electrical properties. Thin films of the polymer sandwiched between two metal electrodes exhibit bi-stable resistance with an ON/OFF ratio exceeding100, good reproducibility and persistence ability. Memristive behavior has been assigned to charge trapping and stabilization of voltage-induced conformational changes by physical crosslinking via hydrogen bonds between amide and carbonyl groups.

Quantum Beats in Transient Absorption of Bis(thienyl)diketopyrrolopyrrole Thin Films

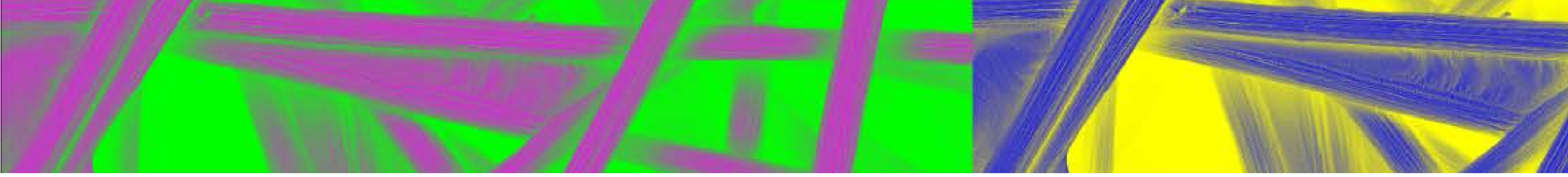
Thottappali M. A., Rais D., Pfleger J.

Abstract. We studied the initial step of a singlet fission process in bis(thienyl)-diketopyrrolopyrrole thin films using ultrafast transient absorption spectroscopy, and found oscillatory modulations of the signal in the range up to ≈10 ps after photoexcitation. Employing FFT analysis and Raman spectroscopy we assigned these oscillations to the lattice phonons modulation of the coupling of the (S_0, S_1) and (S_1, S_0) states of adjacent, dimer-forming molecules, with their biexciton state (T_1, T_1)

Formation of Transmembrane Pores in Lipid Membranes: Dual(1+) FCS Approach

Sachl R., Cujová S., Vandana, Riegerová P., Kapusta P., Muller H. M., Steringer J. P., Hof M., Nickel W.

Abstract. Pore-forming proteins/peptides often oligomerize on the cellular membrane, which can affect the cell in many ways. Pore formation has several applications one of which is the part of this study is the change in the inner part of vesicles (endosomal and exosomal exchange). My PhD study focuses on pore formation induced by Fibroblast Growth Factor 2 (FGF2). This protein binds PI(4,5)P2 and subsequently oligomerises on the membrane. To correlate FGF2 oligomerisation to trans-membrane pore formation, we developed and used a new dual(1+) FCS approach. This approach's readout parameters are protein oligomeric state, diffusion coefficient and protein surface concentration measured selectively on leaky and nonleaky vesicles, i.e. on the vesicles that do contain pores or on the vesicles that have an intact bilayer. This approach enables us to tell the average number of molecules of FGF2 required to create a pore on vesicles as well as pore size variation with time.



F-5 PHYSICS OF SURFACES AND INTERFACES

Scaling-up of the Epoxy Resin/Graphites Composites Bipolar Plates for PEMFCs

<u>Darabut A. M.</u>*, *Lobko Y., Yakovlev Y., Gamon Rodriguez M., Matolín V.

Abstract. Proton exchange membrane fuel cell (PEMFC) is a notorious technology used as an alternative power source based on hydrogen fuel. The bipolar plates (BPs) are one of the critical components of the PEMFC due to their properties and their high cost of the total PEMFC's cost. One of the most promised types of BPs is polymer composites due to their properties, and low cost. The polymer composites based on the epoxy resin and carbon fillers (commercial natural and synthetic graphite, as well as own-prepared thermally expanded graphite) were prepared by compression molding. The dependence between electrical conductivity and filler content of the composites was shown through the percolation threshold. The scaling-up from the laboratory samples to the BPs with different surface areas was successfully done. The prepared BPs were tested in a real fuel cell station and the performance of membrane electrode assemblies with obtained BPs was studied.

Phosphonic Acid Anchored Porphyrins on Atomically Defined Cobalt Oxide Surfaces: In-situ Infrared Spectroscopy at the Electrified Solid/Liquid Interface

<u>Fusek L.</u>*, *Kastenmeier M., Fromm L., Franz E., Gorling A., Brummel O., Myslivecek J., Libuda J.

Abstract. Organic/inorganic hybrid materials are essential building blocks, e.g., in solar energy conversion and sensor technology. In this work, we anchored 5-(4-phosphonatophenyl)-10,15,20-(triphenyl)porphyrin on atomically defined Co3O4(111) and studied the hybrid interface under electrochemical conditions (aqueous electrolyte, pH10) by IR spectroscopy. The porphyrins bind via the phosphonic acid group to Co2+ ions as chelating tridentates. Observed changes in the binding geometry are fully reversible.

Thermally Stimulated Decomposition of Phenylphosphonic Acid on Cu(111)

***Kalinovych V.**, Piliai L., Kosto Y., Matolinová I., Matolín V., Skála T., Prince K. C., Tsud N.*

Abstract. In the present work, we have studied the adsorption geometry and thermal stability of phenylphosphonic acid (PPA) of 0.1 and 0.2 ML coverage on the Cu(111) single crystal in vacuum by synchrotron radiation photoelectron spectroscopy, resonant photoelectron spectroscopy and near-edge X-ray absorption fine structure spectroscopy. Thermal stability has been investigated in the temperature range from 25 °C to 500 °C. We found that PPA adsorbed on Cu(111) surface in tridentate binding geometry and remained stable up to 300 °C with phenyl ring tilted by 80° with respect to the surface.

PtAu Thin Film Catalyst for Oxygen Reduction Reaction

***Mohandas Sandhya A. L.**, Khalakhan I., Xie X.*

Abstract. Large scale deployment of Proton Exchange Membrane Fuel Cells (PEMFC)in the market is hampered due to several shortcomings among which high platinum catalyst cost and its stability are the most prominent. While technology has started reaching cost-efficiency targets the problem remains with durability because of the significant susceptibility of catalyst to corrosion and deactivation, especially at the cathode side. Recent studies showed the utilization of Au underlayer promotes the stability of the Pt catalyst. The aim of this work was thus to investigate the stabilization effect of Au. Two different systems were investigated: Pt deposited on Au using magnetron sputtering technique and co-sputtered Pt–Au alloy with a low amount of Au. A simulation of the PEMFC operating conditions was performed in an electrochemical cell by employing accelerated degradation tests (ADT) which include potentiodynamic cycling from low to high potentials. The results showed that for Pt on Au system significant segregation of Au atoms to the surface occurs during ADT. This led to a decrease of Pt active surface area. In contrast, co-deposited Pt–Au alloy showed improved stability towards degradation.

Perovskites and Metal Hexacyanoferrates Incorporated with N-doped Carbon Catalysts for Oxygen Reduction Reaction

Nedumkulam H.

Abstract. This work tried to understand the kinetics of ORR using N-doped carbon material incorporated with Lanthanum-based perovskite oxides of first-row transition metals and metal hexacyano ferrates, and also, we tried to understand the role of carbon and nitrogen functionality in the mechanism of ORR. After analyzing ORR kinetics of synthesized compounds, we tried to understand how the Nitrogen functionalized PANI-KB improves ORR activity of perovskites. Further the mechanism of ORR was analyzed by hydrogen peroxide reduction reaction (HPRR) and hydrogen peroxide disproportionation studies. The role of Nitrogen-doped carbon material was analyzed by adding PANI-KB with perovskites and found the addition improved onset potential and current density along with the increase in the number of electron transfers during ORR. And also, we have tried to prepare different first-row transition metal hexacyanoferrates incorporated with carbon-based PANI to improve ORR kinetics of the 2+2 electron pathway.

Effect of Ceria Stoichiometry and Morphology on Gold Nanoparticles in the Model Au/CeO_2 Catalyst for CO Oxidation Reaction

Piliai L.,Vorokhta M., Matvija P., Skála T., Khalakhan I., Matolínová I.

Abstract. The high prospect of using cerium-based gold nanoparticles as catalysts in C1 chemistry for industrial usage attracted much scientific attention, but the complex electronic structure of cerium oxide assumes the difficulties in modelling of its systems and emphasizes on the importance of practical research. With insight to this problem understanding the redox behavior of the gold/ceria system is a considerable step in establishing the mechanisms of its catalytic activity. In this work, we studied the model systems of stoichiometric ceria thin films grown on the single crystal substrate and characterized them with Resonance Photoelectron Spectroscopy (RPES), Near-Ambient Pressure X-ray photoelectron spectroscopy (NAP-XPS) and Ambient Pressure Scanning Tunneling Microscopy (AP-STM) to determine the oxidation state of the cerium and gold along with changes in their surface morphology within gaseous and vacuum environments. Finally, it was found that reduced ceria as well as ceria with higher number of surface steps promote shift to higher binding energy in gold nanoparticles due to different degree of metal-support interaction and size of the grown nanoparticles.

The Use of Organometallic Functionalized Tips in Scanning Tunneling Microscope

Pinar A.

Abstract. Scanning tunneling microscopy (STM) can provide information of the atoms and atomic bonds on a sample by imaging them by means of the quantum tunneling effect. A very sharp metallic tip is brought close to the surface of interest, and applying bias voltage the electron tunneling current can be controlled and measured. This can provide information about the spatial and electronic configuration of the specimen as a local probe with atomic resolution. The presentation will focus on the use of organometallic molecules as functionalized tips to acquire special features to study magnetic properties like Kondo effect and spin flip.

A Study on the Influence of CeO_2 Particle Size in CeO_2/Pt(111) Inverse Model Electrocatalyst on its Electrochemical Stability

Samal P. K., Fusek L., Keresteš J., Khalakhan I., Myslivеček J.

Abstract. In this study, inverse model CeO_2/Pt(111) electrocatalysts have been prepared in UHV at different oxidation temperatures and characterized using surface science techniques XPS, STM, AFM and LEED. Cyclic voltammetry in alkaline solution indicates a pronounced structure sensitivity in the electrochemical stability of CeO_2 nanoparticles. Large CeO_2 nanoparticles with compact step edges show better stability at the potential of hydrogen evolution reaction compared to relatively smaller CeO_2 nanoparticles with open step edges.

Preparation and properties of Pt/Co_3O_4(111) thin film catalyst

Uvarov V., Samal P. K., Mysliveček J., Johanek V.

Abstract. Model system of Pt nanoparticles on well-ordered cobalt oxide thin film was investigated as a potential (electro)catalyst, using X-ray photoelectron spectroscopy (XPS), diffraction (LEED) and microscopy (STM). Pt growth was monitored from very small coverages (leading to atomic dispersion) and relation between Pt oxidation state and structure of Co_3O_4 support is discussed. Thermal stability and catalytic properties of Pt/Co_3O_4 and pristine Co_3O_4 were characterized by XPS and thermal desorption (TPD).

F-6 Quantum Optics and Optoelectronics

Charge Transport in Halide Semiconductors

Betušiak M.

Abstract. Halide semiconductors gained a lot of attention for their interesting optoelectronic properties. The performance of every semiconductor device is strongly tied to crystal defects. However, halide semiconductors have dynamic defect structure and often display ionic conductivity that impede thorough defect characterization. In this work, we study defects employing the time-of-flight method (Laser-induced Transient Current Technique) while focusing on the suppression of the ionic drift.

Thin Epitaxial Films of CeO_2 for Optics and Opto-electronic Applications

Hrabovsky J., Kubat J., Myslivecek J., Veis M.

Abstract. This study deals with complex studies of magneto-optical (MO) response of epitaxial thin films of solid, Co-doped, reduced ceria and pure ceria. Thin films were characterized by XPS, LEED, STM, spectroscopic ellipsometry and measurement of MO activity. The work focuses on studying MO response of the films depending on film thickness, cobalt concentration, oxidation state of cerium and chemical state of cobalt. Spectra of MO response consist of low energy region where the MO activity is mediated by transitions from defect induced states to conduction band and high energy region where a peak of MO activity appears which we attribute to transitions from valence band to conduction band. In this work we qualitatively explain the effects of the physico-chemical states of the thin films on the structure of the obtained MO spectra, mainly on the appearance of the MO activity in the low energy region, and on the changes of the position of the MO peak. Compared to other preparation methods the epitaxial thin films allow achieving a shift of the MO peak in the direction of higher photon energy.

Optical Gating of Epitaxial Graphene Grown on 6H Silicon Carbide Substrate

Morzhuk B.

Abstract. Different and original approach to the effective gating of epitaxial graphene grown via thermal decomposition from 6H silicon carbide substrate is offered. It is based on a controlled variation of graphene sheet conductivity by optical excitation of semi-insulating SiC substrate. Simple graphene field effect transistors were fabricated, their spectral photoresponse of source-drain current under quasi-monochromatic light was studied and photothermal ionization spectroscopy was performed.

High Harmonic Generation in Nanostructures

Peterka P.*, *Kozák M.

Abstract. High harmonic generation is a strongly non-linear phenomenon which enabled the emergence of attosecond physics. The discovery of generating high harmonics in solids opens the way for their amplification in nanostructures. Numerical calculations by the Finite-difference time-domain method allows to determine and optimize the field strength factor in nanostructures, which is important for efficient generation of high harmonics.

Crucible Initialization and Enhancement for Graphene Growth

Shestopalov M.

Abstract. Using crucibles as fabricated for graphene growths leads to sample contamination. As fabricated crucibles are not quenched respectively to conditions which they are going to be annealed during regular growth, carbon from crucible's surface can sublimate and affect the process. Preventing carbon's sublimation without applying any negative effect is the main goal. Also walls of crucible could be covered by Silicon containing compounds to decrease rate of carbon sublimation.

F-8 Atmospheric Physics, Meteorology and Climatology

Sensitivity of Secondary Inorganic Aerosol Concentrations to Precursor Emissions and Inorganic Aerosol Modules in CAMx over Central Europe

***Bartík L.**, Huszár P., Vlček O., Eben K.*

Abstract. This presentation briefly summarizes both current knowledge about secondary aerosol (SA) gained from its observations and advances in approaches to its modeling in state-of-the-art models. Furthermore, the ideas of planned simulations, the aim of which will be to improve model prediction of SA over Central Europe, as well as the results of simulations focused on inorganic SA and their comparison with measurements, which represent the starting point for the planned simulations, are presented.

Projected Climate Change Indices over Prague Using CMIP5

Dhib S.

Abstract. The main objective of this study is to estimate changes in climate characteristics for rainfall and temperature in Prague, based on calculation of 9 relevant climate indices using 3 models, 3 scenarios. Historical and two future periods are under consideration. The study concludes, a high decrease in the cold days (frost and ice), the number of tropical nights increase five times more, and an increase by about 30 days of very heavy rainy days by RCP 8.5 scenario during the period of 2081–2100.

Modeling the Contribution of Regional Wind-blown Dust Emissions to Urban and Rural PM Levels over Central Europe

***Liaskoni M.*, Bartik L., Huszar P.**

Abstract. Wind drag causes the disintegration of material from the Earth's surface leading the fluxes of both fine and coarse particle matter into the air increasing background PM concentrations especially over (semi-)arid areas. Here we provide a model-based estimate of the regional impact of PM emissions from wind erosion (wind-blown dust — WBD) on urban and rural PM levels for a central European domain (9 km resolution) and a nested domain over Czechia (3 km resolution) using a well-established windblown dust module (called "WBDUST") for the 2018–2019 period. As driving meteorological data, we used WRF simulations. The obtained emission fluxes were comparable to anthropogenic ones indicating the great importance of windblown dust even over such non-arid areas. WBD emissions were implemented into the CAMx chemistry transport model and we performed simulations with and without these emissions. Our results showed that both urban and rural PM levels are significantly higher if wind-blown dust is considered.

Urban Climate: A Literature Review

Radović J.

Abstract. This presentation is a brief literature review made for several topics closely related to the Urban Climate (UC). At first, the urban area and its influence on the atmosphere above are presented along with some of the main issues we are dealing with while trying to understand what is happening in the cities. Along with the mentioned, the issue of Urban Heat Island (UHI) is addressed. After that, the literature review on the Computational Fluid Dynamic Models (CFD) specifically used for UC studies is presented, together with the latest improvements made in The Parallelized Large-Eddy Simulation Model (PALM) and PALM for Urban Applications (PALM4U) model studies. The presentation is rounded by pointing out some of the main ideas on how to have better approach to the UC studies and what can we expect in the future regarding it.

Localized Seasonal to Decadal Climate Prediction — Downscaling in High Resolution over Central Europe

Shilenje Z.W.

Abstract. The future of global climate prediction applications depends among others on how well it can be used on smaller temporal and spatial scales. Actually, global climate models (GCMs) can predict the climate system with some benefits given by proper initialization for seasonal up to about decadal scale over global to regional spatial scales often spanning hemispheric circulation patterns, continents, or regional blocks. These GCMs are too coarse when applied to much smaller or localized geographical areas such as individual countries or regions with complex topography. This has led to localization of climate predictions through down-scaling techniques using regional climate modes (RCMs) in high resolution. Seamless regional climate prediction in temporal framework of seasons to decades become an important aspect for direct use of climate information in decision making for this time span if well understood. The main aim of this study is to downscale climate prediction on seasonal to decadal scales for Central Europe. The study will, therefore, present the possible regional climate change projections using RCMs and the added value for near term prediction over the region.

F-9 PARTICLE AND NUCLEAR PHYSICS

Search for New Physics with the ATLAS Detector

Biroš M.**, **Řezníček P.

Abstract. Interactions between elementary particles are well described by the Standard Model of particle physics. However, number of experiments observing discrepancies between theory and experiment gradually rises. One of the most promising clues to new physics beyond Standard Model can be hidden in properties of B-mesons. This work relates to the angular analyses of the final-state particles of the rare Bd to K∗(892) muon muon decay and of the decay of Bs to J/psi phi with the ATLAS detector in Run 2.

Geodesic Paths in the Lipkin–Meshkov–Glick Model

Matus F.

Abstract. We study geodesics on the parameter manifold for systems exhibiting first and second order quantum phase transitions for a particular version of the Lipkin–Meshkov–Glick model, as a protocol to optimize the task of adiabatic ground-state preparation in a fixed amount of time. The coupled nonlinear geodesic equations are solved numerically for a finite number of qubits. We also study the metric tensor properties, which from its definition, it has been recognized that it has a divergent behavior at points in parameter space that induce level-crossings. Those points are shown to cause that geodesics will not always be an optimal protocol.

F-12 Physics Education and General Problems of Physics

Physics Education in Upper Secondary Schools

Pschotnerova P.

Abstract. The paper presents the literature search from the first year of my doctoral studies. The aim of the literature search was to find out how physics is taught at upper secondary schools in the Czech Republic, how the Matura examination in physics looks like in the Czech Republic, and to map how the results of physics education are obtained at the end of upper secondary schools in chosen countries.

F-13 Physics of Nanostructures

Mixed Dimensional Metallophtalocyanine-2D Material Heterojunctions

Degtev I.

Abstract. Mixed dimensional heterojunctions composed of zero-dimensional (0D) magnetic organic molecules deposited on two-dimensional materials (2D) is a promising basis for the fabrication of future spintronic and optoelectronic devices. At present work heterostructures made of metallophtalocyanine (MPc) molecules and transition metal dichalcogenides (TMDC) were prepared and investigated; an example case: CoPc/MoS2 will be presented. The obtained samples were characterized by optical microscopy, atomic force microscopy (AFM), and polarized Raman and photoluminescence spectroscopy. The variation of the MoS2 optical properties due to the interaction with the CoPc will be discussed.

Structural and Optical Study of Zinc Sulphide Quantum Dots

Gupta S.

Abstract. Undoped ZnS QDs, Vanadium doped ZnS QDs, and Manganese doped ZnS QDs were synthesized using co-precipitation method. P-XRD was used to confirm phase of the samples, supported by SAED. Calculated crystallite size was found to be 1.7–2.3 nm, exhibiting strong size confinement, confirmed using HRTEM. UV–Visible absorption spectroscopy patterns of the samples exhibited blue-shift compared to bulk material, and energy band gap in the range of 3.9–4.1 eV was found using Tauc plots. PL emission spectroscopy patterns confirmed the existence of surface defects in the synthesized QDs.