Laboratory of Aerosols Chemistry and Physics

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Main fields of research

- Atmospheric aerosols
- Indoor/outdoor aerosols
- Nucleation phenomena
- Engineered nanoparticles and health
- Aerosol technology
- Density functional study of interfacial phase transitions and nanodrops
- Dynamic properties of simple and complex fluids on a molecular scale
- Molecular simulations and perturbation theories for model fluids and fluid mixtures
- Development of equations of state based on molecular theory
- Molecular simulations of solid–liquid interfaces
- Mesoscale simulations of polymeric and energetic systems
- Density functional study of interfacial phase transitions and critical phenomena at non-planar surfaces
- Dynamic non-equilibrium properties of complex fluids and their mixtures

Research projects

Molecular-level simulations aqueous electrolytes

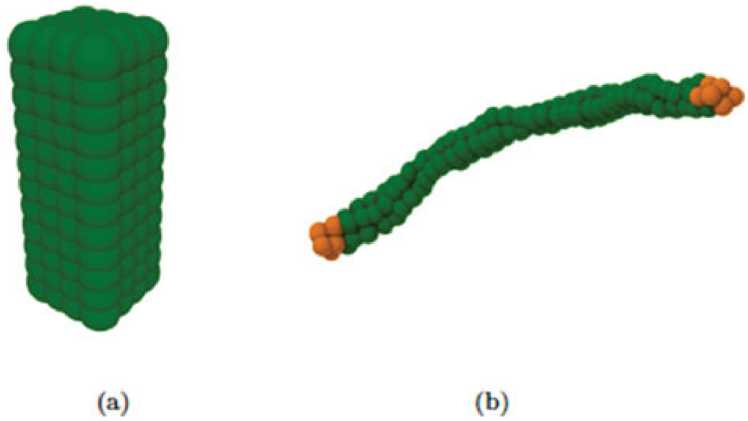
(I. Nezbeda, ivonez@icpf.cas.cz; joint project with the University of Ontario, Institute of Technology, Oshawa, ON, Canada and UJEP; supported by UJEP)

This project deals with common non-polarizable models of electrolytes with the goals to (i) assess their appropriateness, (ii) find ranges of their applicability, and (iii) examine the possibility of their improvement by a reparametrization. Consistency tests of available literature data for the chemical potential were also performed. All simulations used the recently developed MPM-MC method demonstrating thereby its efficiency. [Ref. 3]

Tailored self-assembly of polyelectrolyte copolymers with surfactants in aqueous solutions

(Z. Posel, M. Lísal, posel@icpf.cas.cz, lisal@icpf.cas.cz; supported by GACR, project No. 13-02938S)

Multidisciplinary study of the tailored self-assembly of branched polyelectrolyte copolymers with surfactants in aqueous solutions aimed at deeper understanding of the relationship between the chain architecture and the structure, stability, thermodynamic behavior and properties of nanostructures formed under different conditions (pH, ionic strength, temperature) was carried out. A combination of dissipative particle dynamics and newly developed hybrid Monte Carlo method with experiments was used. [Refs. 11, 15, 24, 27]



Schematic of the meso-scale models: (a) parallepepid model P with 192 *p*-type beads (green) and (b) elongated model L with 136 *p*-type beads and 16 *k*-type beads (orange)

A controlling of diffusion processes in pores with varying permeability

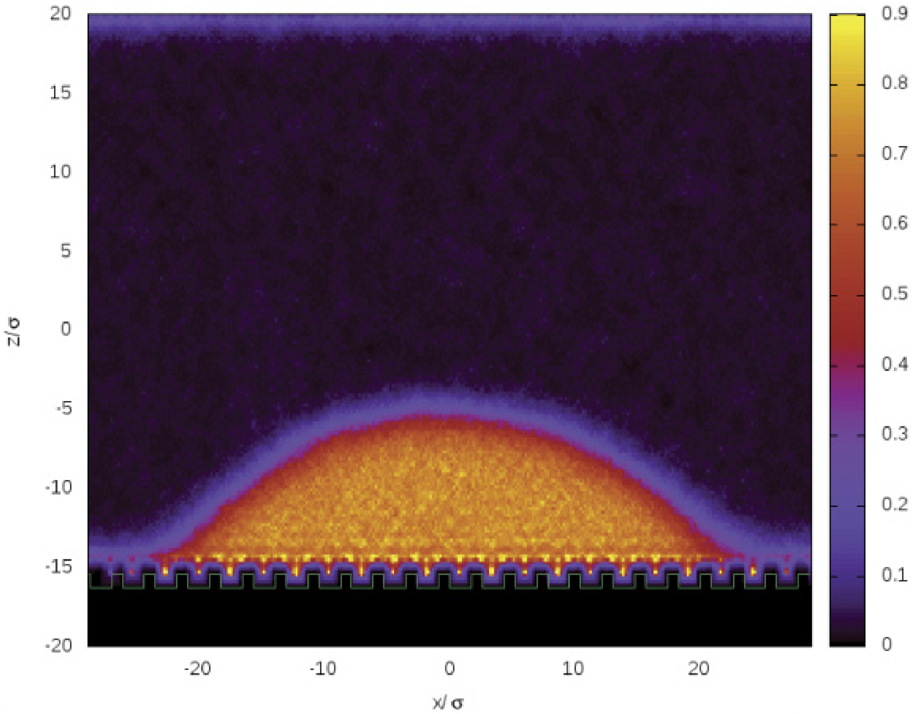
(A. Malijevský, M. Lísal, malijevsky@icpf.cas.cz, lisal@icpf.cas.cz; supported by GACR, project No. 13-09914S)

Interfacial phase transitions at non-planar surfaces have been studied in the framework of a density functional theory and effective Hamiltonian theory. New hidden connections (covariances) between adsorption phenomena at different substrate geometries have been found and explained. While most of the results obtained by the two theories give mutually consistent conclusions, the molecular-based density functional theory whose implementation was newly extended for the geometries possessing nontrivial symmetries, provides a more microscopic insight into the understanding of the interfacial phenomena and revealed some new and surprising predictions. These results are not only interesting by their own rights but also serve as a pre-requisite for a further study of dynamical properties of fluids (such as diffusive processes) at modified surfaces and between patterned walls. [Refs. 16, 17]

Mesoscopic modeling of protein - surface interactions

(A. Malijevský, Z. Posel, and M. Lísal, malijevsky@icpf.cas.cz, posel@icpf.cas.cz, and lisal@icpf.cas.cz; supported by Grant Programme of the MEYS, project No. LH12020)

Mesoscopic modeling using dissipative particle dynamics was employed to systematically study the effect of shape, size and hydrophobicity / hydrophilicity of proteins on their adsorption kinetics. Mesoscale models of proteins and surfaces were obtained from atomistic simulations of individual proteins in water and individual proteins close to walls using mapping from the atomistic to mesoscopic level. [Refs. 11, 17]



Two-dimensional density profile of liquid droplet on the molecularly rough surface

Maximizing the EU shale gas potential by minimizing its environmental footprint (ShaleXenvironmenT)

(M. Lísal, lisal@icpf.cas.cz; supported by EU HORIZON2020, project No. 640979)

Securing abundant, affordable, and clean energy remains a critical scientific challenge. Fortuitously, large shale formations occur within Europe. As the conventional gas production in Europe peaked in 2004, European shale gas could become a practical necessity for the next 50 years. However, the exploitation of shale gas remains challenging. Further, its environmental footprint is at present poorly quantified. Great care is needed to assess and pursue this energy resource in the safest possible way for the long-term future of Europe whilst protecting the European diverse natural environment.

With this in mind, ShaleXenvironmenT assembled a multi-disciplinary academic team, with strong industrial connections. The primary objective is to assess the environmental footprint of shale gas exploitation in Europe in terms of water usage and contamination, induced seismicity, and fugitive emissions. Using synergistically experiments and modeling activities, ShaleXenvironmenT will achieve its objective via a fundamental understanding of rock-fluid interactions, fluid transport, and fracture initiation and propagation, via technological innovations obtained in collaboration with industry, and via improvements on characterization tools. ShaleXenvironmenT will maintain a transparent discussion with all stakeholders, including the public, and will suggest ideas for approaches on managing shale gas exploitation, impacts and risks in Europe, and eventually worldwide. The research will bring economical benefits for consultancy companies, service industry, and oil and gas conglomerates. The realization of shale gas potential in Europe is expected to contribute clean energy for, e.g., the renaissance of the manufacturing industry.

Human EXposure to Aerosol COntaminants in Modern Microenvironments

(V. Ždímal, zdimal@icpf.cas.cz; supported by EC, Marie Curie Actions - Initial Training Networks, project No. 315760, FP7-PEOPLE-2012-ITN, HEXACOMM)

The main research goal of HEXACOMM is to apply scientifically-based modelling and experimental methods to relate concentrations of particulate matter in the indoor domestic environment to its sources and human exposure implications. The second research objective is to determine the human exposure arising from such exposure at both individual and collective (population) scales at modern microenvironments.

Contributions from outdoor air will be taken into account. Central idea of HEXACOMM is that a combination of tools and methods will enable us to relate indoor air quality to aerosol contaminants in urban homes, offices, vehicles with human exposure in a quantitative manner. To achieve our goal and objectives we propose to undertake, in parallel, a carefully designed validation programme at the European scale combining specifically targeted indoor air quality measurements, source apportionment studies, micro-environmental modelling, dosimetry modelling and exposure studies. Ultimately, our vision is that such enhanced understanding of the underpinning science will lead to improved indoor air quality in European domestic environments, while facilitating development of strategies to mitigate the impacts of aerosols on human exposure. [Refs. 2, 5, 6]

Aerosols, Clouds, and Trace gases Research InfraStructure Network

(V. Ždímal, zdimal@icpf.cas.cz; supported by EC, project No. INFRA-2010-1.1.16 ACTRIS)

ACTRIS (Aerosols, Clouds, and Trace gases Research InfraStructure Network) is the European Project aiming at integrating European ground-based stations equipped with advanced atmospheric probing instrumentation for aerosols, clouds, and short-lived gas-phase species. ACTRIS will have the essential role to support building of new knowledge as well as policy issues on climate change, air quality, and long-range transport of pollutants.

ACTRIS is building the next generation of the ground-based component of the EU observing system by integrating three existing research infrastructures: EUSAAR, EARLINET, CLOUDNET, and a new trace gas network component into a single coordinated framework. ACTRIS is funded within the EC FP7 under “Research Infrastructures for Atmospheric Research”.

Aerosols, Clouds, and Trace gases Research InfraStructure Network

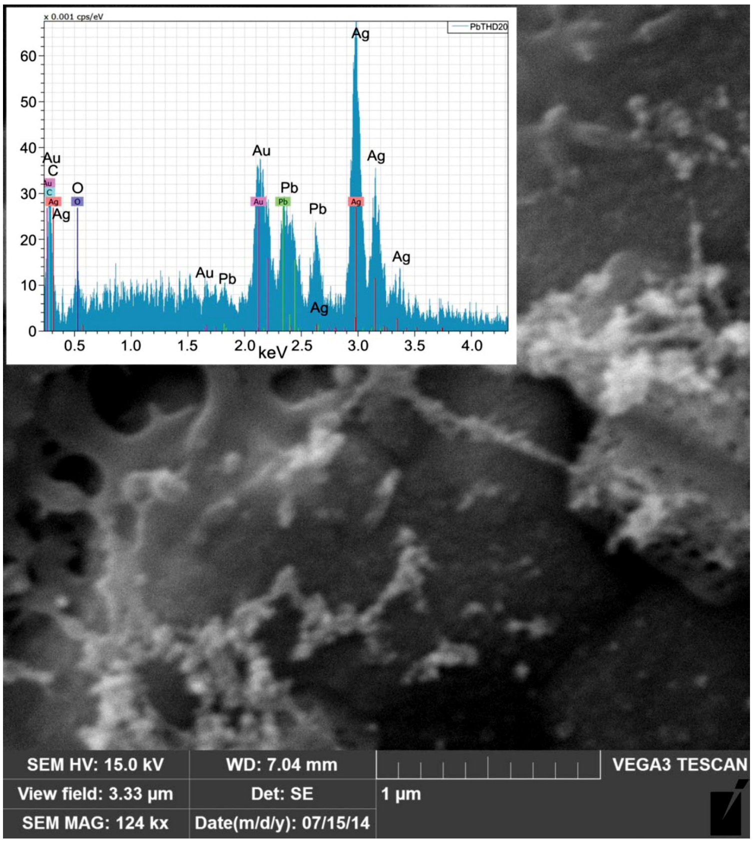
(V. Ždímal, zdimal@icpf.cas.cz; supported by EU HORIZON 2020, project No. 654109, ACTRIS-2 IA)

Detecting changes and trends in atmospheric composition and understanding their impact on the stratosphere and upper troposphere is necessary for establishing the scientific links and feedbacks between climate change and atmospheric composition. The primary objective of ACTRIS is to provide the 4D-variability of clouds and of the physical, optical and chemical properties of short-lived atmospheric species, from the surface throughout the troposphere to the stratosphere, with the required level of precision, coherence and integration. The second objective is to provide effective access to this information and the means to more efficiently use the complex and multi-scale ACTRIS parameters serving a vast community of users working on models, satellite retrievals, and analysis and forecast systems. The third objective is to raise the level of technology used in the RI and the quality of services offered to the community of users, involving partners from the private sector. Finally, the fourth objective of ACTRIS is to promote training of operators and users and enhance the linkage between research, education and innovation in the field of atmospheric science.

Centre for studies on toxicity of nanoparticles

(P. Moravec, moravec@icpf.cas.cz; supported by GACR, project No. P503/12/G147)

The rapid expansion of nanomaterials production and their use in many products create a need for understanding the mechanisms of nanomaterial interactions with living systems. This need is above all given by unique properties of nanoparticles related to their dimensions and by their ability to penetrate into various tissues and cells in organism. Nanoparticles are also formed unintentionally as a result of the anthropogenic activities (industry, local heating). The proposed interdisciplinary centre of basic research will integrate laboratories capable to perform complex studies on mechanism of the toxicity of important and widely used engineered nanoparticles, as well as anthropogenic nanoparticles in the environment with a special attention paid to heavily polluted areas of the Czech Republic. The studies will be performed on thoroughly characterized nanoparticles to obtain valid and comparable results on biological action and toxicity of nanoparticles. [Refs. 10, 13, 22, 23]



SEM image and EDS spectrum of the sample of NPs synthesized by oxidation of PbTHD2 at T_R = 480 °C, Q_R = 1400 cm^3/min, P_{PbTHD2} = 2.20 Pa, and c_O = 5 vol. %

Methodology of evaluation of air quality effect on library and archival collections

(J. Smolík, smolik@icpf.cas.cz; supported by the Ministry of Culture of the CR, project No. DF11P01OVV020)

The aims of the project are: a) development of evaluation methods for indoor air quality in libraries and archives, targeted at reduction of damages on library and archival collections caused by adverse effects of environment and b) gaining detailed knowledge of direct dependences between damage of library and archival collections and surrounding environment, leading to precautions reducing the adverse effects of deteriorated environment. [Refs. 1, 9]

International co-operations

Imperial College London, London, UK: Confined fluids
Penn State University, State College, PA, USA: Dissipative particle dynamics simulations of adsorption behavior of model proteins on surface
University of Loughborough, Loughborough, UK: Dynamic density functional theory
University of Ontario Institute of Technology, Oshawa, ON, Canada: Macroscopic and molecular-based studies in the statistical mechanics of fluids
U.S. Army Research Laboratory, Weapons and Materials Research Directorate, MD, USA: Mesoscale simulations of energetic and reactive materials
Finnish Meteorological Institute, Helsinki, Finland: Studies on homogeneous nucleation using diffusion chambers
Laboratory of Atmospheric Chemistry, Paul Scherrer Institute, Switzerland: Source apportionment from highly time-resolved data.
Norwegian Institute for Air Research, Kjeller, Norway: Indoor aerosol behavior
Technical University of Crete, Chania, Greece: Aerosols in the indoor environment
Technical University of Denmark, Lyngby, Denmark: Indoor air and aerosols
University of Helsinki, Division of Atmospheric Sciences, Helsinki, Finland
University of Vienna, Faculty of Physics, Dept. of Aerosol physics and Environmental Physics, Vienna, Austria: Black and elemental carbon analysis, aerosol optical properties

Visits abroad

D. Brus: Finnish Meteorological Institute, Helsinki, Finland (12 months)
M. Cusack: University of Birmingham, Birmingham, UK (1 month)
A. Malijevský: Imperial College London, London, UK (1 month)
N. Talbot: IDAEA- CSIC, Barcelona, Spain (3 months)
N. Zíková: Clarkson University, NY, U.S.A. (5 months)

Publications

Original papers

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