

Structure and Dynamics of Meso-Bio-Nano Systems



Researchers

A. Yakubovich, G. Sushko, A. Verkhovtsev, M. Hanauske, C. Kexel and Prof. Andrey Solov'yov

Principal Investigator

Prof. Andrey Solov'yov

Project Term

2012 - 2014

Project Areas

Statistical Physics, Soft Matter, Biological Physics, Nonlinear Dynamics

Clusters

LOEWE CSC Cluster Frankfurt

Institute

Frankfurt Institute for Advanced Studies

University

Goethe Universität Frankfurt am Main

Introduction

Biological matter, as well as any complex form of inanimate matter, consists of many different components linked by numerous, different interactions. Important efforts in deepening of our molecular-level understanding of biological systems and their dynamical behavior concern the origin, nature and evolution of various complex molecular systems and processes, as well as the emergence of new features, properties, functions in the systems with increasing their complexity. On the meso- and nanoscales, the physics and chemistry of biological macromolecules and atomic clusters typically deal with such behavior. Many examples of the emergence of qualitatively new features can be quoted, e.g. the development of new collective properties when going from small molecules to large clusters or the cluster aggregation on surfaces leading to the appearance of fractally shaped morphologies.^[1] The fractal morphologies, being emerged in dynamical systems on the nanoscale, remain characteristic for many systems, including biological ones, at practically all larger scales, and are present in practically all living systems.

Methods

The project „Structure and dynamics of Meso-Bio-Nano systems“ was carried out under the supervision of Prof. Dr. Andrey V. Solov'yov at the Frankfurt Institute for Advanced Studies. The project was devoted to investigation of structure formation and dynamics of animate and inanimate matter at the micro- and nanometer scales. There are many examples of complex many-body systems of micro- and nanometer scale size exhibiting

unique features, properties and functions. These systems may have very different natures and origins, e.g., atomic and molecular clusters and nanoparticles,^[2,3] nanostructures,^[4] biomolecules,^[5] and mesoscopic systems.^[6,7]

A detailed understanding of the structure and dynamics of these systems on the nanometer scale is a difficult and fundamental task, the solution of which is necessary in numerous applications of nano- and biotechnology, material science^[8,9] and medicine.^[10] Although mesoscopic, nano- and biomolecular systems differ in their nature and origin, a number of fundamental problems are common to all of them. Seeking answers to the fundamental questions is at the core of a field entitled Meso-Bio-Nano (MBN) Science which is a new interdisciplinary field that lies at the intersection of physics, chemistry, and biology.

Outlook

The MBN Science bundles up several traditional disciplines such as theoretical atomic and molecular physics, condensed matter physics, solid state physics, quantum physics, and chemistry, classical, quantum, and statistical mechanics, physical kinetics, molecular biology, biochemistry, and biophysics. A detailed theoretical description and complete understanding of MBN systems and phenomena with their involvement can only be achieved by utilizing a wide range of theoretical approaches and methods known from all these disciplines combined with advanced computational techniques and with the use of powerful computers.

Reference

- [1] I.A. Solov'yov, N. Solov'yov, A. Kebaili, N. Masson, and C. Brechignac (March 2014), Thermally induced morphological transition of silver fractals, *Physica Status Solidi B*, 251 (3): 609-622. <https://doi.org/10.1002/pssb.201349254>
- [2] A.V. Yakubovich, G. Sushko, S. Schramm, and A.V. Solov'yov (July 2013), Kinetics of liquid-solid phase transition in large nickel clusters, *Physical Review B*, 88 (3): 035438-(1-9). <https://doi.org/10.1103/PhysRevB.88.035438>
- [3] A.V. Verkhovtsev, A.V. Korol, and A.V. Solov'yov (October 2013), Quantum and classical features of the photoionization spectrum of C60, *Physical Review A*, 88 (4): 043201-(1-8). <https://doi.org/10.1103/PhysRevA.88.043201>
- [4] P. Moskovkin, M. Panshenskov, S. Lucas, and A.V. Solov'yov (July 2014), Simulation of nanowire fragmentation by means of kinetic Monte Carlo approach: 2D case, *Physica Status Solidi B*, 251 (7): 1456-1462. <http://dx.doi.org/10.1002/pssb.201350376>
- [5] S.N. Volkov, E.V. Paramonova, A.V. Yakubovich, and A.V. Solov'yov (January 2012), Micromechanics of base pair unzipping in DNA duplex, *Journal of Physics: Condensed Matter*, 24 (3): 035104-(1-6). <https://doi.org/10.1088/0953-8984/24/3/035104>
- [6] G.B. Sushko, V.G. Bezchastnov, I.A. Solov'yov, A.V. Korol, W. Greiner, and A.V. Solov'yov (November 2013), Simulation of ultrarelativistic electrons and positrons channeling in crystals with MBN Explorer, *Journal of Computational Physics*, 252: 404-418. <https://doi.org/10.48550/arXiv.1307.6771>
- [7] G.B. Sushko, A.V. Korol, W. Greiner, and A.V. Solov'yov (June 2013), Sub-GeV electron and positron channeling in straight, bent and periodically bent silicon crystals, *Journal of Physics: Conference Series*, 438: 012018-(1-11). <https://doi.org/10.48550/arXiv.1307.6787>
- [8] A.V. Yakubovich, A.V. Verkhovtsev, M. Hanauske, and A.V. Solov'yov (August 2013), Computer simulation of diffusion process at interfaces of nickel and titanium crystals, *Computational Materials Science*, 76: 60-64. <http://dx.doi.org/10.1016/j.commatsci.2012.12.039>
- [9] A.V. Verkhovtsev, G.B. Sushko, A.V. Yakubovich, and A.V. Solov'yov (October 2013), Benchmarking of classical force fields by ab initio calculations of atomic clusters: Ti and Ni-Ti case, *Computational and Theoretical Chemistry*, 1021: 101-108.
- [10] E. Surdutovich, A.V. Yakubovich, and A.V. Solov'yov (February 2013), Biodamage via shock waves initiated by irradiation with ions, *Scientific Reports*, 3: 1289-(1-6). <https://doi.org/10.1038/srep01289>

Last Update: 2022-06-30 23:19