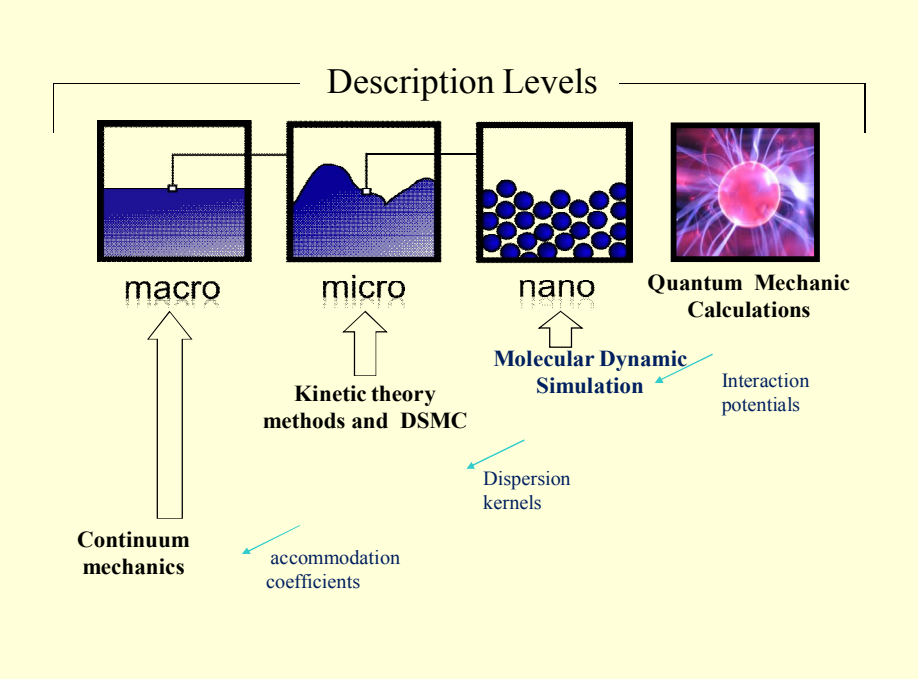
Multiscale Modeling Of Physicochemical Processes

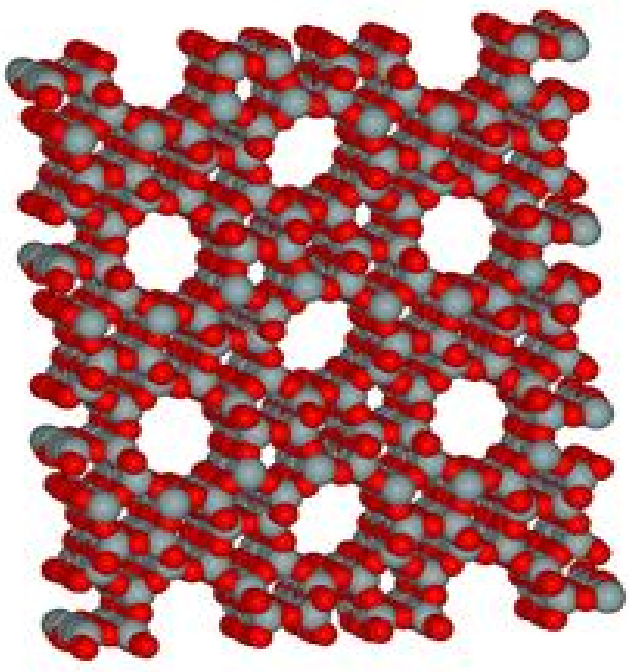
(prof. Kovalev V.L.)

Prospects for development of science-intensive industrial sectors demand to carry out new researches of physicochemical processes in extreme conditions and in the design of new materials. The development of predictive modeling at an atomic-molecular level is becoming particularly relevant in recent time. Nowadays such approaches have become possible due to improvements in modern supercomputer technologies.

Multi-disciplinary basic researches of phenomena and processes are being conducted within the framework of this scientific direction. They include construction of new multiscale models, development of new computing algorithms for their investigation and making calculations using multinuclear massively-parallel computation systems. The general mathematical approaches and cooperation of specialists in mechanics, mathematics and quantum chemistry make possible to investigate urgent applied problems of various physicomechanical nature on different spatial and time scales.

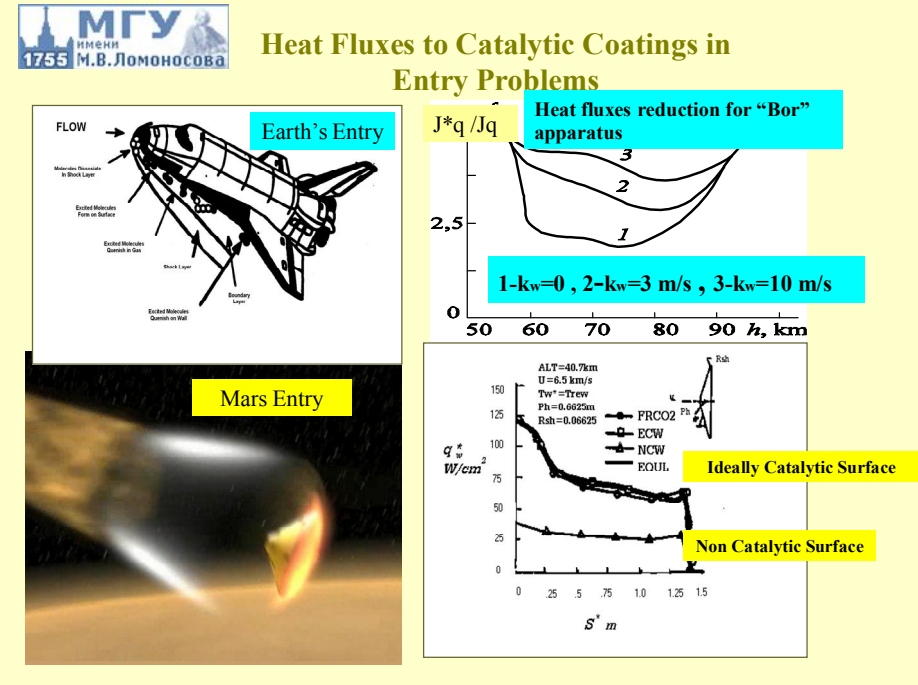


One of the numerous problems here (in this scientific direction) is connected with multiscale modeling of gas and fluid currents at catalytic surfaces. It includes currents in channels and pores of sorption and catalytic materials taking in account molecular structure and topological and structural material peculiarities.



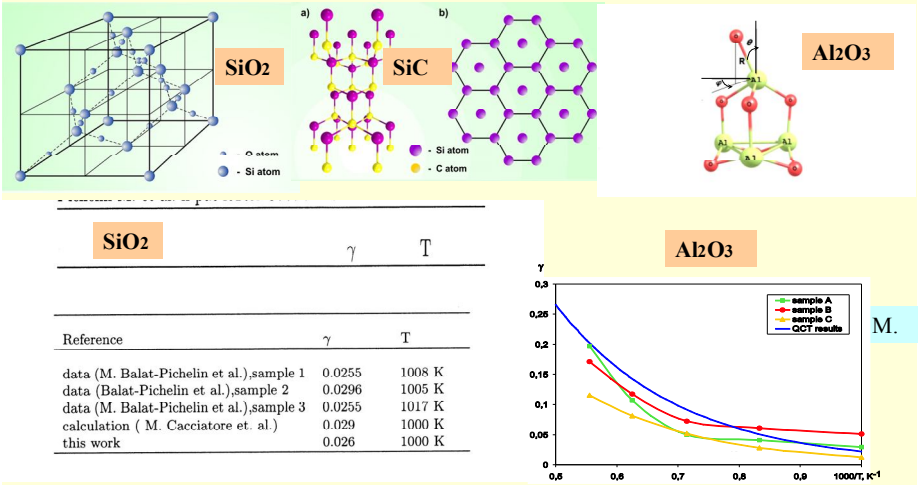
Zeolites are molecular sieves

The analysis of interaction of gas phase molecules with different material surfaces is also used in rarefied gas aerodynamics problems which have gradually rising scientific and practical interest due to aerospace technology development. In addition, the investigations of catalytic properties of reusable spacecrafts (space shuttles) heat-shielding coverings remain urgent because catalytic processes give more than half of heat flux to body surface in hypersonic flow.



New materials, including nanostructured heat-shielding materials, are developed for perspective hypersound aircrafts. Such materials should provide thermal protection at surface temperatures about 2000 K and higher. The most recent approaches based on quantum mechanics and molecular dynamics can help you to understand the mechanism of heterogeneous catalytic processes, to analyze their elementary stages and estimate the influence of spatial structure of surface-layer on catalytic phenomena. To find a mechanism of heat-transfer processes and determine their key features is an important task which decision make possible to construct thermal protection of modern spacecrafts more effectively. The theoretical description gives a chance to reduce the size of experimental work necessary for reliable description of heterogeneous catalytic processes on spacecrafts surface.

Predictable simulation of properties of heat-shielding materials based on molecular dynamics and quantum mechanics

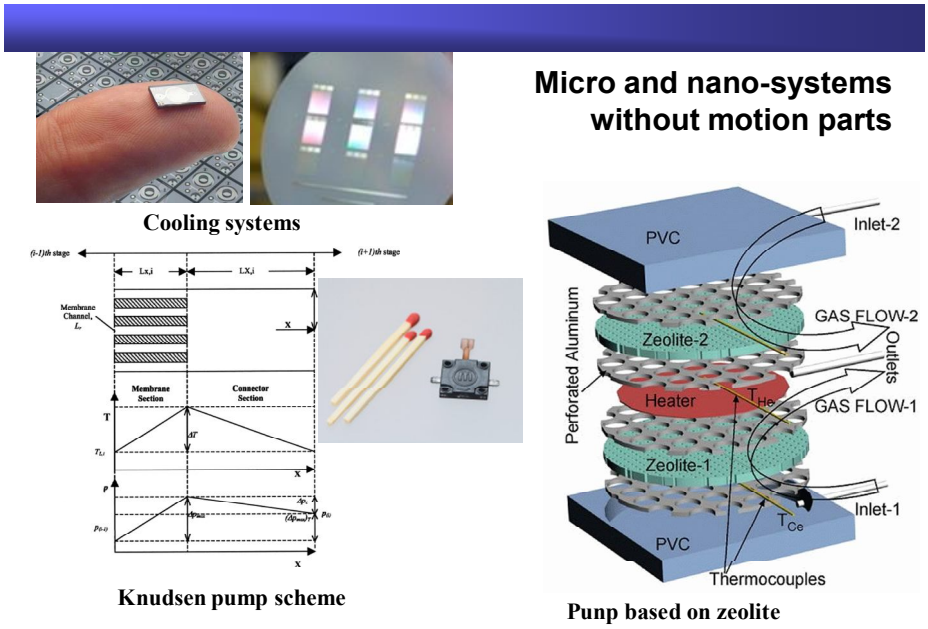


Calculated and measured recombination coefficients of oxygen atoms on SiO2 and Al2O3

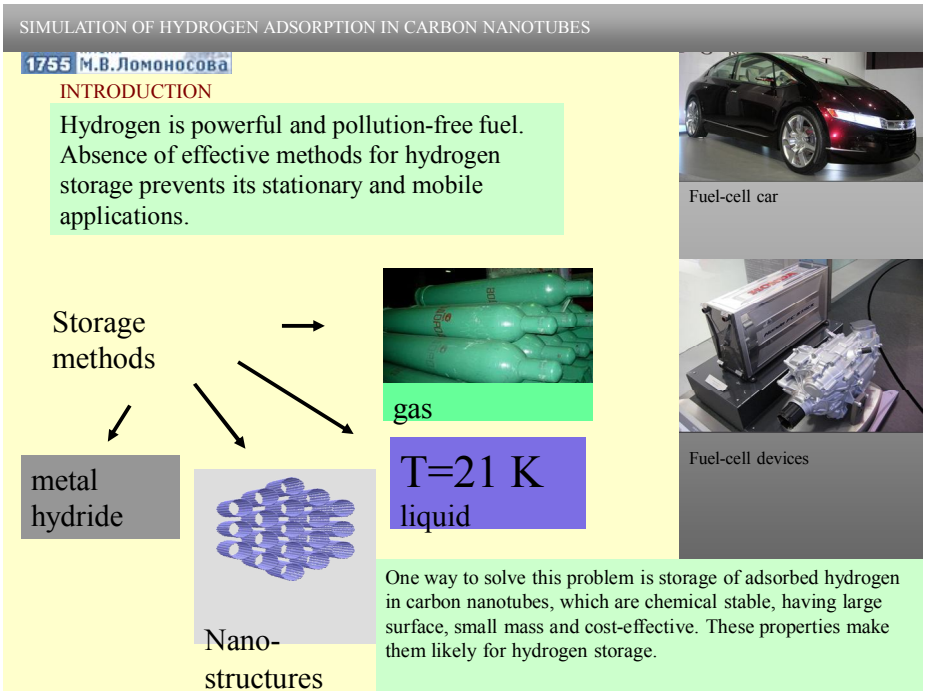
M.

At present the interest to such currents is constantly increasing due to development of micro- and nano-technologies. Particularly using new porous materials in catalytic and sorption processes and in electrotechnical devices puts on agenda the necessity of establishment of quantitative relations between chemical composition and material structure and functional characteristic expected from it. Taking into account these factors is also necessary to define interaction laws between gas and surface in major perspective processes such as catalytic organic synthesis in meso- and nanoporous materials, processes passing in catalytic afterburners based on active nanoparticles, etc. Such analysis demands improvement of models combining various spatial and time scales but allows conducting directed search and design of materials with given set of functional characteristics.

Moreover modern technologies has opened up possibilities for manufacturing various micro- and nano-electromechanical systems (MEMS/NEMS) with unique characteristics such as light(insignificant) weight, low energy/power consumption, high efficiency and sensitivity. Designing a large amount of similar devices is connected with such problems as gas and liquid current, heat transfer processes in micro and nano-structures. Methods of multiscale modeling of currents and physicochemical interactions in micro- and nano-structures and devices taking into account atomic structure of rigid body, chemical properties of gas, thermal motion of atoms on surface, adsorption phenomena, surface roughness and system macro geometry are developed within the framework of this scientific direction.



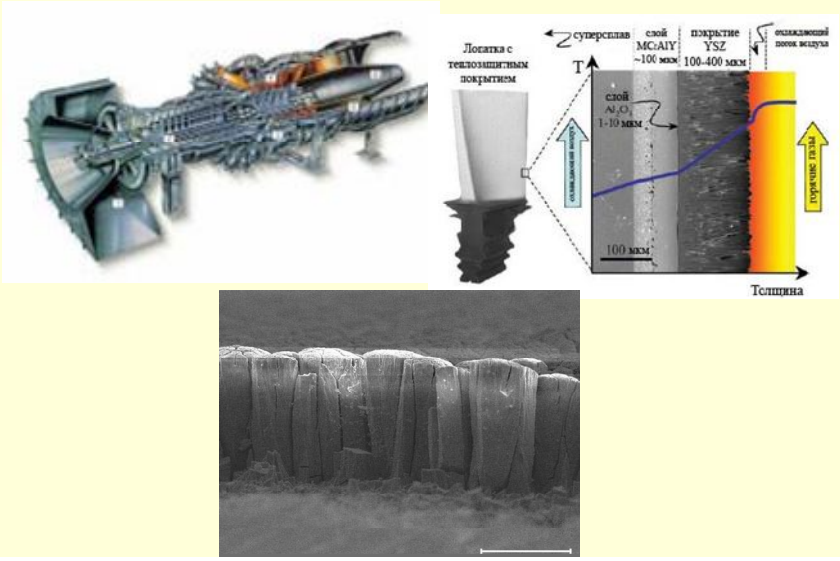
Particularly, the possibilities of effective storage of hydrogen are investigated here. It is important to notice that hydrogen is the most energetically effective and non-polluting gas.



The creation of multilevel models and corresponding program modules for investigating burning processes in combustion chambers and nonequlibrium currents in aviation engine gas turbines is one of the major concrete fundamental problems in this scientific area. The kinetic schemes presenting gross reaction in

terms of set of elementary stages and reliable estimation methods of kinetic characteristics (speed factors, products distribution of elementary stages) are developed.

Creation of heat-shielding coverings on turbojet engine blades



The corresponding algorithms are created for kinetic models verification and optimization of aviation engines work. Also/moreover calculations of three-dimensional nonequilibrium currents in aviation engines basic knots are carried out.