(1) Laboratory of Chemical Cybernetics (Physical Chemistry Division of Chemistry Department of MSU.

Subject: *Molecular modeling of enzymatic and photochemical reactions in biochemical systems*

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Research activities are related to the studies of biochemical processes by means of modern molecular modeling tools. We use various quantum chemical approaches, combined quantum mechanics / molecular mechanics (QM/MM) and molecular dynamics methods. Our current projects include studies of photophysical properties of photoreceptor proteins (flavin containing proteins, members of GFP (green fluorescent protein) family, light-harvesting complex LH1 of bacterial photosystem. Another part of the research is devoted to the enzymatic reactions (hydrolysis in GTPases, proteolysis in matrix metalloproteinases *etc*.) and related drug design.

(2) Laboratory of Molecular Spectroscopy (Laser Chemistry Division of Chemistry Department of MSU; in collaboration with Laser Center, University of Latvia, Riga)

Subject: *The optimal optical cycles for ultracold molecule production: the modelling based on highly accurate spectroscopy and ab initio calculation*

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The laser production and manipulation of the ultracold molecular assembles is greatly facilitated by accurate knowledge of the structure, dynamic, magnetic and electric properties of the electronic states involved. In spite of the recent progress in the systematic spectroscopic investigation of the promising diatomic species such as alkali metal dimers the reduction of the raw experimental data available for excited electronic states to precise structure (potential and interaction matrix elements) and radiative (transition dipole moments and Einstein coefficients) parameters is very challenged and still unambiguous procedure.

We deal with the rigorous physical models and numerical recipes currently developed for the comprehensive deperturbation treatment of for fully mixed and regular perturbed alkali diatomic states in a wide range of excitation energy and internuclear distance. The crucial role of high accurate *ab initio* calculations on the spin-orbit and angular coupling matrix elements in the deperturbation analysis is demonstrated. The homogeneous perturbation effect on nodal structure of the multi-components wave functions and relevant overlap integrals are considered.

(3) Laboratory of Laser Diagnostic (Laser Chemistry Division of Chemistry Department of MSU)

Subject: *Qualitative and Quantitative Analysis of Environmental Samples by Laser-Induced Breakdown Spectrometry*

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Laser-Induced Breakdown Spectroscopy (LIBS) is one of the most promising techniques for direct rapid atomic emission analysis applicable for the field analysis. The focused high-power laser radiation produces laser plasma on the surface or in the volume of any material. Characteristic emission of atoms and ions in plasma allows quantitative and qualitative analysis of liquids, gases, and solids. The main advantages of LIBS are absence of a sample preparation, a small amount of an evaporated sample (up to 1 ng), local and remote analysis of light and heavy elements. The peculiarity of this technique is the use of short-lived plasma source with relatively high electron density (up to 1020 cm^{-3}). Thus, the following aspects of the technique should be taken into account: (i) Stark effect is a dominant mechanism for line broadening in emission spectra, (ii) spectral interferences are larger than in other atomic emission techniques due to Stark effect, (iii) sensitivity is often insufficient to determine traces due to small amount of sampled material. Our research area is the increasing of sensitivity and accuracy of LIBS. We can suggest several topics for undergraduate student research:

1. *Experimental determination of the Stark broadening parameters of iron atomic lines in laser-induced plasma.* This is a fundamental study to measure Stark broadening parameters, which are needed to simulate the emission spectra of non-LTE plasmas. Such a kind of plasmas is of interest for astrophysical researches or the studies of low-density plasmas (glow discharge, hollow cathode discharge etc.)The laser-induced plasma is useful

plasma source for Stark parameters measurements due to a wide range of available electron density.

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2. *Determination of alkaline earth metals ratios in seawaters by Laser-Induced Breakdown Spectroscopy.* Changes in atmospheric CO_2 (which is extremely important for carbon cycle study) may have been driven by variables in carbonate deposition, chemical weathering, and hydrothermal activity. Precise and continuous records of seawater alkaline earth metals ratios may be able to constrain relative changes in the above processes. LIBS can provide a unique opportunity for *in-situ* measurements of Mg, Ca, Sr and Ba in seawater. At the same time, the Ba and Sr contents are low due to low solubility of their sulfates.

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3. *The effect of compression degree of powdered manganese nodules on the Fe / Mn signal ratio in laser-induced plasma.* Iron-Manganese nodules (IMN) are often considered as perspective source of manganese. The main characteristic of IMN is Fe / Mn ratio. Moreover, the mechanism of their formation is very important for geochemistry and petrology. Therefore the spatial distribution of Fe / Mn ratio over nodule is of particular interest. The local analysis can be easily performed by LIBS, but the matrix effect can influence the analysis. The matrix effect caused by different degree of compression will be considered in this study.

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(4) Laboratory of Laser Spectroscopy (Laser Chemistry Division of Chemistry Department of MSU)

Subject: First principle based modeling of superheavy element chemistry

Supervisor: Andrei Zaitsevskii, Dr. Sci. (Hab.), principal researcher at the Laser Spectroscopy Laboratory

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Superheavy nuclides with atomic numbers Z = 112 – 117 (i.e. in the range that is characteristic for the island of stability) are being successfully synthetized in Flerov Laboratory of Nuclear Reactions (JINR, Russia), RIKEN Nishina Center for Accelerator-

Based Science (Japan), Oak Ridge National Laboratory (USA) etc. These nuclei have sufficient lifetimes to enable the studies of the chemical reactions of the latter. At present, the yield of superheavy elements is very small, about one atom per week (atom-at-a-time regime), and up to now, gas thermochrogratography remains the only experimental technique successfully applied to investigate the chemistry of elements with Z = 112 and more. The only physical / chemical property that can be determined this way is the adsorption energy. Electronic structure modeling of superheavy element compounds is a much more universal source of information on physical and chemical properties of the elements from the island of stability, offering the possibility to predict various characteristics of their compounds.

New electronic structure modeling technologies developed in course of our collaboration with the Laboratory of Quantum Chemistry of Petersburg Nuclear Physics Institute have enabled us to build models yielding superheavy element adsorption energies in a quantitative agreement with the available experimental data; the results of thermochromatographic experiments for some elements from the island of stability have been predicted. Systematical calculations of simple compounds of these elements with common light elements provided insight into specific manifestations of the periodic law related to the unprecedented role of the effects of relativity. One can note, for instance, the subperiodic structure of the seventh period and striking differences between Cn and Fl and their homologues. In contrast, the changes of properties in passing from “normal” heavy elements to the elements of the island of stability in groups 1 and 2 are regular, so that elements 119 and 120 are alkaline and alkaline earth metals respectively.

Nowadays both experimental and theoretical studies are focused on the chemistry of element 113, the only non-inert element of the unique short subperiod composed of this element and flerovium. Its atomic configuration, a single p electron outside of the stable (in a sense, rare-gas-like) closed shell, has no analogs in the periodic table. We have already shown that its chemistry should be radically different from that of its formal homologue, thallium. Furthermore, the hydroxide of E113 has good chances of becoming the first experimentally detected gas-phase compound of an element from the island of stability, and we had obtained very accurate estimates for various properties of this compound.

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