Laboratory of theoretical physical chemistry
Jiri Vanicek, Assistant Professor
EPFL-SB-ISIC-LCPT, BCH 4312, Lausanne, CH-1015
jiri.vanicek@epfl.ch

Master projects

For a more detailed description of the projects, contact Prof. Jiri Vanicek directly.

1) Development of efficient time-dependent semiclassical techniques to describe quantum chemical dynamics

Example: **Calculation of photodissociation cross-sections**

Even with the fastest supercomputers, accurate real-time *quantum dynamics* is only feasible for systems with a few atoms. This is due to the exponential growth of the computational cost with the number of atoms. One can avoid this trap by using approximate, but often very accurate *semiclassical* techniques. The standard approach to semiclassical description of, e.g., *photodissociation spectra* is the use of periodic orbit theory in the energy domain. The goal of this project is to implement a more natural and accurate novel semiclassical algorithm in the time domain and compare it with the exact quantum and classical cross-sections. On the way, the student will become familiar with the classical, semiclassical, and quantum-mechanical methods in chemical dynamics.

2) Description of quantum nuclear effects on properties of molecules at finite temperature using path integral molecular dynamics

Example: **Calculation of thermodynamic and kinetic isotope effects**

Most present-day *molecular dynamics* (MD) simulation packages for description of molecular properties are based on an (exact or more often approximate) quantum-mechanical treatment of the electronic degrees of freedom, but only on a classical treatment of nuclei. Therefore they completely ignore quantum nuclear effects. For reactions in which hydrogen plays a central role, this approach often gives results far from reality. This can be best seen by the measurement of the *isotope effects*, in which the hydrogen is replaced by deuterium. Results of classical MD calculations are very different from accurate quantum calculations and from the experiment. For thermodynamic properties, quantum nuclear effects can be treated by the so-called *imaginary-time path-integral* methods which have been recently implemented into several molecular dynamics packages. The goal of

this project will be to develop an understanding of the *path integral molecular dynamics* (PIMD) and use the AMBER implementation of PIMD to calculate quantum corrections to the thermodynamic and kinetic isotope effects on several reactions.

3) Using statistical biophysics to predict functional RNA-RNA interactions

Example: **Prediction of microRNA targets in viruses and humans**

Only a small fraction of the human genome codes for proteins. It was long thought that the remaining DNA is “junk DNA,” but in last several years, many new noncoding genes were discovered in this poorly understood region. Among them are the *microRNAs* – short noncoding RNA molecules that regulate coding genes by inhibiting translation. Since the detailed biochemical mechanism of the *target selection* is not known, one has to devise probabilistic methods that circumvent this lack of information. The goal of the project will be to extend existing algorithms and/or develop new algorithms for target selection and apply them to predict microRNA targets in viruses and humans. Among the techniques used will be statistical thermodynamics and bioinformatics.