Ph.D. positions in theoretical chemical physics and bioinformatics

The Chemical Physics Theory Group of Prof. Jiri Vanicek at the Swiss Federal Institute of Technology in Lausanne (EPFL) invites applications for Ph.D. positions in theoretical chemical physics and in bioinformatics. One position will be a part of the Swiss National Centre of Competence for Research (NCCR) "*Molecular Ultrafast Science and Technology"*. The start date is flexible, but should be in **2012**. Research projects are in the following three areas:

1) Development of efficient and accurate first-principles **quantum** and **semiclassical methods** to describe quantum dynamical properties of molecules, clusters, and mesoscopic systems. Applications include calculations of *ultrafast time-resolved electronic and vibrational spectra* using quantum dynamics including *nonadiabatic transitions, spin-orbit couplings, and explicit coupling to a time-dependent electromagnetic field.* One part of the project will be combining the dynamical methods with *on-the-fly ab initio* calculation of the electronic structure.

2) Development of **quantum-statistical** methods to describe physical properties of molecules, clusters, and mesoscopic systems. This will also involve efficient computational implementation of the theory, using, e.g., Path Integral Monte Carlo or Path Integral Molecular Dynamics. Applications include the calculation of *quantum reaction rates*, *kinetic isotope effects* on chemical reactions in solution, and of other quantum thermodynamical properties. Part of the project will be combining the dynamical methods with *on-the-fly ab initio* calculation of the electronic structure.

3) Development of algorithms based on **classical statistical physics and bioinformatics** for predicting interactions between biologically important molecules. Applications include *prediction of mRNA targets regulated by microRNAs*, of *transcription factor binding sites*, and of *protein-protein interactions*.

Requirements:
1) An excellent academic record.
2) An M.S. or M.A. in physics, chemistry, mathematics, or a related field. (Exceptional candidates with a four-year B.A. or B.S. degree will be considered.)
3) Proficiency in written and spoken English.
4) Proficiency in writing computer codes in C, C++, or Fortran 90.

See http://lcpt.epfl.ch for more information about our group. Interested candidates should submit an application including a curriculum vitae, list of publications, copy of a transcript, contact information of three references, and a description of research interests. Applications should be sent by e-mail to jiri.vanicek@epfl.ch or by post to Prof. Jiri Vanicek, EPFL SB ISIC LCPT, BCH 3110, CH-1015 Lausanne, Switzerland. These positions **require** acceptance to the EPFL doctoral program, for which online applications must be filed **simultaneously** at http://phd.epfl.ch/edch.