UNIVERSITY of ROCHESTER

DEPARTMENT OF CHEMISTRY
***Oleg Prezhdo**, Professor of Chemistry*
Fellow of the American Physical Society
Senior Editor of the Journal of Physical Chemistry

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POSTDOCTORAL SCHOLAR POSITIONS
THEORETICAL AND COMPUTATIONAL CHEMICAL PHYSICS

Postdoctoral positions are immediately available in the theory group of Professor Oleg Prezhdo.

(A) Excited State Dynamics in Nanoscale Materials.
Time-domain, atomistic simulation of excitation and electron transfer, electron-phonon relaxation, spin dynamics and related processes on nanoscale, including molecule-bulk interfaces, semiconducting and metallic quantum dots, carbon nanotubes and graphene nanoribbons, as motivated by photovoltaics, molecular electronics, spintronics, ultrafast spectroscopies, DNA sequencing, laser therapies, etc.

(B) Non-Adiabatic Molecular Dynamics and Time-Dependent Density Functional Theory.
Development and implementation of NAMD and TDDFT algorithms with the aim at the applications described in (A). Fundamental aspects of semiclassical physics, coupling of quantum and classical (or semiclassical) dynamics, system-bath interactions.

(C) Forces in Biology.
Phenomenological modeling and molecular dynamics simulation of force-induced processes in biology as studied by atomic-force microscopy, optical tweezers and related experiments. Biological catch-bond.

Interested candidates should submit their CVs, including a list of references to
oleg.prezhdo@rochester.edu

1. O. V. Prezhdo “Photoinduced dynamics in semiconductor quantum dots: insights from time-domain ab initio studies”, *Acc. Chem. Res.*, **42**, 2005 (2009).
2. O. V. Prezhdo, Y. V. Pereverzev, “Theoretical aspects of the biological catch-bond”, *Acc. Chem. Res.*, **42**, 693 (2009).
3. O. V. Prezhdo, W. R. Duncan, V. V. Prezhdo, “Dynamics of the photoexcited electron at the chromophore-semiconductor interface”, *Acc. Chem. Res.*, **41**, 339 (2008).
4. O. V. Prezhdo, “Quantized Hamilton dynamics”, *Theor. Chem. Acc.*, vol. "New Perspectives in Theoretical Chemistry", **116**, 206 (2006).
5. C. F. Craig, W. R. Duncan, O. V. Prezhdo “Trajectory surface hopping in the time-dependent Kohn-Sham theory for electron-nuclear dynamics”, *Phys. Rev. Lett.*, **95** 163001 (2005).
6. Y. V. Pereverzev, O. V. Prezhdo, L. R. Dalton, “Macroscopic order and electro-optic response of dipolar chromophore-polymer materials”, *ChemPhysChem*, **5** 1821 (2004).

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