Combining DFT and TDDFT Approaches with XAS for Biological and Environmental Sciences

X-ray absorption spectroscopy (XAS) has become an essential tool for scientists investigating the fate of contaminants and nutrients in soils, sediments, surface waters and marine settings by providing information on the chemical form of these elements. Density functional theory (DFT) and molecular dynamics-based modeling, when combined with XAS, enables identification of chemical species in heterogeneous settings and opens the pathway to identify mechanisms by which contaminants and nutrients are transformed in solution and at natural interfaces.

SLAC National Accelerator Laboratory invites, effective immediately, applications for a 2-year theoretical post-doctoral fellow (PD) position in the Structural Molecular Biology (SMB) group at the Stanford Synchrotron Radiation Lightsource (SSRL). The PD will work closely with SSRL staff and a team of scientists from DOE-BER’s Environmental Molecular Sciences Laboratory (EMSL) to apply theoretical tools towards the interpretation and analysis of X-ray spectroscopy datasets. Through this effort, the PD will collaboratively assist the environmental community in utilizing combined spectroscopy and computational analysis to enhance understanding of key biogeochemical processes that control the speciation, distribution and fate of contaminants and nutrients.

To help achieve this goal, the PD will work with biogeochemical researchers on hard X-ray spectroscopy beamlines in defining theoretical studies, performing preliminary theory calculations at SSRL and where needed, writing access proposals for the high-performance computing system at EMSL. The PD will collaboratively participate in data analysis and interpretation through the publication of the work in peer-reviewed scientific journals.

The PD will also assist in developing training material for the SSRL user community to lower the barrier of entry to DFT/TDDFT-based data analysis tools.

Required Qualifications
A Ph.D. in inorganic, geochemical, bioinorganic/biomimetic chemistry, or environmental sciences with strong focus on developing or applying theoretical tools for molecular level interpretation of spectroscopy data.

Experience with DFT and TDDFT methods for the modeling of spectroscopy data (preferably X-ray absorption spectroscopy data) is a must, including demonstrated ability in data analysis, modeling and interpretation of EXAFS data and its correlation to electronic structure from XANES and other spectroscopic techniques.

1. Knowledge of how electronic properties tune spectral shapes and the ability to translate this knowledge to molecular level interpretation is preferred.
2. Understanding and demonstrated knowledge of molecular dynamics methods is a plus (but not in lieu of DFT expertise).
3. Willingness to learn and bridge knowledge/experience gaps.
4. Ability to work independently and in a team environment.
5. Strong organizational skills is a must.
6. Ability to work and communicate effectively with a diverse population; good interpersonal skills are essential.
7. Effective multitasking skills and the ability to switch between several scientific projects.
8. Ability to interact and communicate with non-experts in theory applications is essential.
9. Effective written and verbal communication skills.
If you are a postdoctoral researcher ready to test your talents in this field of research and hone your skills at a national laboratory widely recognized for its work in the physical, chemical, and environmental sciences, we want to connect with you. SLAC is committed to fostering a work environment that promotes inclusion, diversity, equity and accountability. We encourage all qualified applicants to apply; you do not need to meet all the Preferred Qualifications to be considered.

Please send a letter with CV and list of publications to Dr. Ritimukta Sarangi, email: ritis@slac.stanford.edu