Combining Computational Approaches with XAS for Biological and Environmental Sciences

X-ray absorption spectroscopy (XAS), by virtue of its element selectivity and sensitivity to local structure, 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 classical molecular dynamics-based molecular 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, in a close collaboration with DOE-BER’s Environmental Molecular Sciences Laboratory (EMSL), invites, effective immediately, applications for a 2-year theoretical post-doctoral fellow (PD) position. Through this effort, the postdoctoral researcher will collaboratively apply computational tools to biogeochemical systems and develop methods to combine 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 postdoctoral researcher will work with biogeochemical researchers in defining theoretical studies and performing them on the high-performance computing cluster at DOE-BER EMSL laboratories. The postdoctoral researcher will also collaboratively participate in data analysis and interpretation through the publication of the work in peer-reviewed scientific journals. This postdoctoral position will be based at SLAC National Accelerator Laboratory.

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 in the application of density functional theory (DFT) and time-dependent density functional theory (TDDFT) methods for the modeling of spectroscopy data (preferably X-ray absorption spectroscopy) is a must.

1. Understanding and demonstrated knowledge of molecular dynamics methods is a plus (but not in lieu of DFT and TDDFT expertise).
2. Ability to work independently and in a team.
3. Willingness to learn and bridge knowledge/experience gaps and strong organizational skills.
4. Effective written and verbal communication skills.
5. Present research at technical conferences and program/project review meetings.

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 required qualifications listed.

Please send a letter with CV and list of publications to Dr. Niri Govind (niri.govind@pnnl.gov) and Dr. Ritimukta Sarangi, email: (ritis@slac.stanford.edu)