Job Description

Job Title	Post Doctorate RA - Computational Catalysis and Separations Science
Job ID	311228
Location	PNNL - Richland, WA
Full/Part Time	Full-Time
Regular/Temporary	Temporary

Return to Previous Page   Switch to Internal View

Organization and Job ID

Job ID: 311228
Directorate: Physical & Computational Sciences
Division: Physical Sciences
Group: Basic/Applied Molecular Found

Job Description

As a postdoctoral researcher in the Basic and Applied Molecular Foundations (BAMF) group, you will join a talented, multi-investigator team to explore the theory and molecular simulation at complex vapor-liquid, vapor/solid, liquid-liquid or solid-liquid interfaces. The research will be conducted with a combination of electronic structure, molecular dynamics (MD) and data science-based methods. You will be mentored by prominent researchers, in addition to mentors Roger Rousseau and Vanda Glezakou, as you develop a line of computational research. Experience in both classical and ab initio MD fields is highly desirable. The successful candidate will be required to conduct large-scale computer simulations on massively parallel high-performance computing platforms of reactivity and transport at liquid interfaces. The candidate will also interact closely with experimentalists at PNNL who will be performing concurrent measurements on these materials. The programs that the candidate will be contributing to are related to renewable energy practices, such as conversion of chemicals from biomass derived broths, CO_2 capture materials and design of novel ion separation membranes.

- Conduct independent research and work on team assignments
- Lead manuscript development and maintain a strong overall publication record in the peer-reviewed scientific literature
- Interact, communicate, and problem solve with a diverse team of research staff within the BAMF group, PSD and across PNNL
- Present research at technical conferences and project/program review meetings
- Participate in the development of research proposals

Minimum Qualifications

Candidates must have received a PhD within the past five years (60 months) or within the next 8 months from an accredited college or university.

Preferred Qualifications

- Strong verbal and written communications skills.

- Experience with electronic structure and atomistic simulations codes are imperative. Candidates with good knowledge of ab initio molecular dynamics codes, classical molecular software and experience with quantum chemical software, is desirable.

- Programming skills (Fortran, C, C++), theory development and experience with modern high-performance computation platforms are essential for a successful appointment.

- Additional expertise in statistical analysis of data, raining of neutral networks and other machine learning methods would be beneficial and desirable.

- The successful candidate will be asked to work on chemical problems for which a background in physical chemistry can be an asset.

- PNNL offers a culturally and technically diverse environment for collaborative research which bridged disciplines. The successful candidate should be able to work well in a diverse team setting as she/he will interact with both theory and experimental colleagues on collaborative projects in which communications skills are a plus.

PhD. In Chemistry, Physics or Engineering

Equal Employment Opportunity

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Return to Previous Page   Switch to Internal View