Postdoctoral positions in Computational Chemistry

University of California
Campus: San Diego

Academic Department / Research Unit:
San Diego Supercomputer Center

Disciplinary Specialty of Research:
Computational Chemistry, Theoretical Chemistry, Molecular Dynamics, Machine Learning, High-Performance Computing, Atmospheric Chemistry, Computational Molecular Biology, Enzyme catalysis, Heterogeneous Catalysis

Description:
Two postdoctoral positions in Computational Chemistry funded by the National Science Foundation and the National Institutes of Health are available in the group of Dr. Andreas Goetz at the San Diego Supercomputer Center. The research focus of the group is the development and application of molecular simulation methods and software for high-performance computing platforms based on quantum and classical molecular mechanics, statistical mechanics, and machine learning, with applications in biophysics, atmospheric chemistry, and catalysis. The successful candidates will work on one or more of the following three research projects:

1) The Goetz group is part of the NSF Center for Aerosol Impacts on Chemistry of the Environment (CAICE, https://caice.ucsd.edu), a multi-institution, interdisciplinary research center with headquarters at UC San Diego. The goal of CAICE is to understand fundamental processes regarding the chemistry of aerosol particles and their impact on the environment. The postdoctoral scientist will develop highly accurate many-body potentials based on correlated electronic structure reference data and machine learning techniques for atmospherically relevant molecules and their interactions with aqueous aerosol particles containing ions and surfactants. The newly developed potentials will be applied to the computational modeling of gas scattering and reactive uptake of atmospheric gases to sea spray mimics. Molecular dynamics simulations with rare events sampling methods will be used to access structural, thermodynamic, and spectroscopic properties from small model clusters to condensed phase systems with explicit liquid-gas interfaces. Chemical reactions will be studied using quantum chemistry, molecular dynamics, and QM/MM models. The research is highly interdisciplinary, with numerous opportunities to interact with other excellent theoretical and experimental groups within CAICE.

2) Cytochrome c oxidases (CcOs) are redox driven proton pumps in the membranes of mitochondria and many aerobic bacteria that drive ATP synthesis by producing the required electrochemical potential gradient across the membrane. We employ density functional theory (DFT) calculations and classical and QM/MM molecular dynamics simulations to provide a detailed mechanistic understanding of the catalytic reaction pathways and mechanisms of proton pumping in CcO. The postdoctoral scientist will develop Amber force field parameters for redox states of enzyme cofactors along the reaction cycle based on DFT reference data. The new force field will be used in MM and QM/MM molecular dynamics simulations of CcO with advanced sampling protocols to identify water and proton transport pathways and mechanisms and key

residues for proton pumping in CcO. This project is jointly funded and involves close collaboration with Professor Louis Noodleman at Scripps Research.

3) Computer simulations are important to gain a molecular level understanding of catalytic biomass conversion to liquid fuels and raw materials for the chemical industry. In this context we have recently developed a new force field for water over a Pt(111) surface (GAL17). The postdoctoral scientist will extend GAL17 to molecules with functional groups that are relevant for catalytic biomass processing such as carbohydrates and incorporate it into the Amber molecular dynamics software. Molecular dynamics simulations will be performed to investigate water and substrate structure at the metal/liquid interface and to determine solvation free energies along catalytic reaction paths that are obtained from DFT calculations. This project involves close collaboration with the Theoretical Chemistry group at the École Normale Supérieure de Lyon and may involve travel to Lyon in France to facilitate collaboration.

Successful candidates will join a dynamic research environment at the San Diego Supercomputer Center, with access to many additional scientific and career/life opportunities in the broader San Diego research community. The candidates are expected to prepare peer-reviewed manuscripts and attend conferences. We also encourage candidates to prepare fellowship applications. The candidates will receive mentoring to prepare them for future careers in academia or industry, including project management skills, proposal writing and effective scientific communication.

Location:
Nestled along the Pacific Ocean, just steps from the beach and minutes from beautiful downtown La Jolla, ranked among the ten best public universities in the nation and is recognized by the international community for its outstanding achievements in research and development, UC San Diego (https://www.ucsd.edu) offers an exceptionally beautiful and stimulating work environment. As a national leader in computational science and engineering, the San Diego Supercomputer Center (https://www.sdsc.edu) houses advanced computing and networking resources and conducts research in computing technologies and computational sciences. The successful candidates will reside in the new building of the San Diego Supercomputer Center on the main campus of UC San Diego.

Salary and Benefits:
Salary commensurate with UC salary scale including full benefits, see https://postdoc.ucsd.edu/appointment-guidelines for details.

Application Procedure:
Please email Andreas Goetz (agoetz@sdsc.edu) with any questions and to apply. Email applications should include i) a cover letter that summarizes past research and explains how research interests and career goals fit with the lab projects, ii) CV with complete publication list, iii) 2 letters of reference or contact information for at least 2 references.

Qualifications Required
The applicants should have, or expect to shortly receive, a doctorate degree in computational, physical, or theoretical chemistry, computer science, physics, or a closely related field. The

successful candidates will be highly motivated scientists with a strong publication record and research experience in quantum chemistry, ab initio or classical molecular dynamics, preferably with a strong background in potential energy surfaces and statistical mechanics. They must be familiar with Linux and should have excellent programming skills including Python, modern Fortran or C/C++. Parallel programming experience and an interest in high-performance computing and machine learning are also desirable. Applicants should enjoy working on challenging and exciting projects together with a team of international experts.

Position Closing Date:
Open until filled.

Appointment Length/Period:
One year, with possibility of renewals, depending on satisfactory performance and availability of funds.

For more information or to apply, please contact:
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