

Post-doc Position in Computational Catalysis at Simon Fraser University, Canada

Job Description Summary

Dr. Siahrostami's Computational Catalysis Group ([COMCAT](#)) in the Department of Chemistry at Simon Fraser University, Burnaby, BC, Canada has an immediate opening for a two-year (1+1) postdoc position. The group focuses on computational catalysis for clean energy related systems. The current focus is on "Power to X and X to Power" where X is a range of valuable chemicals that are key for a sustainable energy society. The project will center on modeling electrocatalytic systems in order to understand the fundamental limitations of present materials and, ultimately, design better ones.

Required Education, Knowledge, Skills, Abilities:

- PhD in Chemistry, Chemical Engineering, Materials Science, Physics or a related discipline.
- Practical knowledge in the field of Computational Catalysis/Materials.
- Practical knowledge in the field of quantum mechanical simulations such as density functional theory (DFT) calculations, molecular dynamics simulations and machine learning in Catalysis/Materials. Proficient experience on using ASE, ab initio quantum mechanical codes such as VASP, Quantum Espresso, and Gaussian are required.
- Previous experience and knowledge of the most common machine learning tools and techniques (e.g. Scikit-learn, TensorFlow) is a plus.
- Previous research experience in theoretical and computational chemistry with a focus on heterogeneous catalysis, electrocatalysis, photocatalysis, or batteries.
- Ability to solve problems in the performance of the simulations.
- Ability to work on and manage parallel projects.
- Ability to interpret/extract physical meanings from the results of the simulations.
- Strong communication skills (oral and written).
- Ability to work effectively in a group as part of the team.
- Work in a collaborative environment, including both theorists and experimentalists.
- Ability to work with minimal supervision using the above knowledge and skills.

Simon Fraser University is located in Metro Vancouver and is consistently ranked as one of the top comprehensive universities in Canada. The Vancouver area is one of the world's most desirable places to live and work in a very diverse community and provides endless opportunities for outdoor activities.

All qualified candidates are encouraged to apply; however, Canadian citizens and permanent residents will be given priority. SFU is an equity employer and encourages applications from all qualified individuals including women, persons with disabilities, visible minorities, Indigenous Peoples, people of all sexual orientations and gender identities, and others who may contribute to the further diversification of the university.

How to Apply: To apply, please send the following documents in a single pdf file to Dr. Samira Siahrostami (ssiahros@sfu.ca) with the subject line "Postdoc Application".

- 1- Your updated CV including full list of publications.
- 2- A compelling cover letter detailing your relevant experience and passion for this position and your envisioned research proposal.
- 3- Contact information for five professional references.