



## PhD Position at the University of Calgary

### Computational Catalysis

In 2016, the University of Calgary was awarded \$75 million, over seven years, from the [Canada First Research Excellence Fund \(CFREF\)](#) for its initiative entitled: “[Global Research Initiative in Sustainable Low Carbon Unconventional Resources](#)”. The goal of this research is to dramatically reduce the impact of energy extraction and energy use on the environment.

As part of the implementation of its GRI scientific strategy and to improve hydrocarbon recovery, while reducing emissions and energy intensity, we are looking to fill a PhD position to apply and develop the state of the art electronic structure simulation tools and analysis to understand, design and discover materials for catalyzing (electro)chemical reactions such as oxygen reduction and evolution reactions, CO<sub>2</sub> reduction reaction, electrochemical synthesis of hydrogen peroxide and so on, which are all important reactions for application in renewable energy technologies and environmental protection.

We seek applications from qualified and motivated scientists with a passion for clean energy and interdisciplinary research. Successful candidates will be required to work within a team environment and so excellent communication skills and the ability to work effectively with a diverse group of interdisciplinary researchers is a must.

### **Qualifications:**

1. A master degree in Chemistry, Physics, Chemical Engineering, Materials Science or related fields.
2. Previous experience in computational chemistry/physics and density functional theory (DFT) is a plus.
3. Good communication skills, ability to work independently and in a team environment, and strong interest in computational catalysis are essential

The PhD position offers a salary of \$25,000 CAD/year, has operating budget, and has guaranteed funding for 4 years.

### **Application details:**

Applications should consist of a current CV, a list of 2-3 referees with contact information and a cover letter indicating which area you are interested in, as well as your availability. Documents should be emailed in a single PDF file to Prof. Samira Siahrostami at [samira.siahrostami@ucalgary.ca](mailto:samira.siahrostami@ucalgary.ca)

The position is available immediately and the search will continue until the team is assembled.

**In assembling the CFREF research teams, aggressive diversity and equity targets are in place and so applications from under-represented groups are especially encouraged<sup>1</sup>.**

To be eligible as a PhD student at the University of Calgary, the candidate must meet Faculty of Graduate Studies minimum admission requirements, as well as the admission requirements specific to the graduate program of interest as the program requirements may call for higher scores, additional documentation and testing. Please review the Faculty of Graduate Studies admission requirements prior to applying for this position.

**Background information**

- (1) Kulkarni, A.; Siahrostami, S.; Anjli, P.; Nørskov, J. K. *Chem. Rev.* **2018**, *118*, 2302-2312.
- (2) Abroshan, H.; Bothra, P.; Back, S.; Kulkarni, A.; Nørskov, J. K.; Siahrostami, S. *J. Phys. Chem. C* **2018**, *122* (9), 4783–4791.
- (3) Siahrostami, S.; Verdager-Casadevall, A.; Karamad, M.; Deiana, D.; Malacrida, P.; Wickman, B.; Escudero-Escribano, M.; Paoli, E. a; Frydendal, R.; Hansen, T. W.; Chorkendorff, I.; Stephens, I. E. L. S.; Stephens, I. E.; Rossmeisl, J. *Nat. Mater.* **2013**, *12* (12), 1137–1143.
- (4) Shi, X.; Siahrostami, S.; Li, G.; Zhang, Y.; Chakthranont, P.; Studt, F.; Jaramillo, T.F.; Zheng, X.; Nørskov, J. K. *Nat. Commun.* **2017**.
- (5) Lu, Z.; Chen, G.; Siahrostami, S.; Chen, Z.; Liu, K.; Xie, J.; Liao, L.; Wu, T.; Lin, D.; Liu, Y.; Jaramillo, T. F.; Nørskov, J. K.; Cui, Y. *Nat. Catal.* **2018**.
- (6) Siahrostami, S.; Li, G.-L.; Viswanathan, V.; Nørskov, J. K. *J. Phys. Chem. Lett.* **2017**, 1157–1160.
- (7) Siahrostami, S.; Jiang, K.; Karamad, M.; Chan, K.; Wang, H.; Nørskov, J. *ACS Sustain. Chem. Eng.* **2017**, *5*, 11080-11085.
- (8) Jiang, K.; Siahrostami, S.; Li, Y.; Lu, Z.; Gardener, J.; Lattimer, J; Stokes, C.; Hill, W.; Bell, D.; Chan, K.; Nørskov, J.K.; Yi Cui, Y.; Wang, H. *Chem* **2017**, *3*, 950-960.

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<sup>1</sup>The University of Calgary recognizes that a diverse staff/faculty benefits and enriches the work, learning and research experiences of the entire campus and greater community. We are committed to removing barriers that have been historically encountered by some people in our society. We strive to recruit individuals who will further enhance our diversity and will support their academic and professional success while they are here; in particular, we encourage members of the four designated groups (women, Aboriginal People, persons with disabilities and members of visible minorities) to apply. All qualified candidates are encouraged to apply; however Canadians and permanent residents will be given priority. To ensure a fair and equitable assessment, we offer accommodation at any stage during the recruitment process to applicants with disabilities. Questions regarding diversity or requests for accommodation can be sent to Human Resources ([hrhire@ucalgary.ca](mailto:hrhire@ucalgary.ca)).