Ph.D. position in DFT calculations of electrochemical conversion of CO_2 to fuel at the University of Iceland

Fully funded Ph.D. scholarship for 3 years from the University of Iceland (UI) has been rewarded for the project "*Designing catalysts for sustainable fuel production*" supervised by Dr. Egill Skúlason, Professor in Chemistry and Chemical Engineering at the UI.

The board of the Doctoral Fund of the UI will only accept an exceptionally qualified student. That means only students with high grades and research experience in their B.Sc. and M.Sc. studies in *chemistry*, *applied physics* or *chemical engineering* from top universities will be considered.

The project involves *density functional theory* (DFT) calculations of electrochemical CO_2 reduction on transition metal/metal oxide surfaces. Recently we have obtained a new insight into this reaction using detailed atomic scale DFT simulations of this process where the applied potential is varied explicitly and energy barriers are calculated for various proton-electron transfer steps towards several hydrocarbons and alcohols (HCAs) [1,2]. These calculations are able to estimate the product distribution as a function of applied potential, pH and the type of metal electrode used as a catalyst. We understand why copper is the only pure metal electrode that can catalyze this reaction into HCAs and why other metal electrodes mainly form CO, formate or H_2. We have also understood how to engineer the catalyst in order to improve the activity and selectivity. The Ph.D. candidate will continue that work and search for improved catalysts with high-throughput screening as well as detailed atomistic modelling of the most promising candidates before they will be tested experimentally. A post-doc in the group will test out experimentally the candidates obtained from this Ph.D. project. The goal of the overall project is to develop specific catalysts that can convert CO_2 selectively into one of the following products; methane, methanol, ethylene, ethanol and propanol, at low applied potentials.

This position is open for applicants with a background in modelling with DFT calculations in the field of catalysis, and preferably with experience of electro-catalysis. We are searching for an outstanding candidate for this position. Besides a strong scientific background it is important that the candidate has a good technical writing ability and verbal communication skills.

Applications should be sent to **egillsk@hi.is** before **22nd Sep 2017** with the subject: **"Application for a Ph.D. position in computational electrochemistry"**. The application should include a CV, a cover letter describing why the candidate should be considered for this position, transcripts of the B.Sc. and M.Sc. courses and grades, and a list of two Professors/advisors that have supervised the student in his/her B.Sc. and/or M.Sc. research project and are willing to provide a letter of recommendation. **Important: The applicant needs to start the position before 1. January 2018 !**

1. "Modeling the electrochemical hydrogen oxidation and evolution reactions on the basis of density functional theory calculations", E. Skúlason, V. Tripkovic, M. Björketun, S. Gudmundsdóttir, G.S. Karlberg, J. Rossmeisl, T. Bligaard, H. Jónsson and J.K. Nørskov, *Journal of Physical Chemistry C*, **114** (2010) 18182

2. "Faraday efficiency and mechanism of electrochemical surface reactions: CO_2 reduction and H_2 formation on Pt(111)" J. Hussain, H. Jónsson, E. Skúlason, *Faraday Discuss.* ***195*** *(2016) 619*