Ph.D. positions at University of Iceland on DFT calculations of electrochemical N_2 reduction reaction

Fully funded Ph.D. scholarships at the University of Iceland for 3 years supervised by Dr. Egill Skúlason, Professor of Chemical Engineering. Two Ph.D. positions are available in theoretical modelling and are supported through a Center of Excellence Grant by the Icelandic Research Fund for the project *"Artificial nitrogen fixation at ambient conditions through rational catalyst design"*. The overall project involves theoretical simulations, catalyst synthesis, electrochemical measurements and chemical analysis of products where a unique system has been developed for an in-line electrochemical testing of ammonia formation from atmospheric nitrogen in aqueous or non-aqueous solutions at ambient conditions. The overall project consists of several students and post-docs working on specific theoretical or experimental projects. Flow of information are required between the groups. The candidates advertised for these positions here will do theoretical calculations and model the electro-catalysis on the same systems investigated experimentally.

The consortium behind this project are leading scientists from universities in Iceland, Denmark, Sweden, UK, US and New Zealand and close collaboration between these academic institutions and two Icelandic spin-off companies, Atmonia and Grein Research, is on-going.

We are seeking exceptionally qualified applicants for these positions. That means only students with high grades and research experience in their B.Sc. and M.Sc. studies in *chemical engineering, chemistry* or *applied physics* from top universities will be considered.

The project involves density functional theory (DFT) calculations and *ab initio* molecular dynamic (AIMD) simulations of the electrochemical N_2 reduction reaction (NRR) on transition metals, metal nitrides, metal oxides and metal sulfides surfaces (*see relevant publications below*). Explicit solvent and electrolyte effects will be included and energy barriers will be calculated for NRR at varying applied potentials and pH values towards ammonia as well as other possible side- or by-products such N_2H_4, NH_2OH or H_2. Close comparison is made with experiments each time and the ultimate goal is to identify new and/or improved catalysts to test experimentally as well as testing out hypothesis coming from the experimental work.

These positions are open for applicants with a background in modelling with DFT calculations and AIMD simulations in the field of catalysis, and preferably with experience of electro-catalysis. 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 **10th of April 2019** with the subject: **"Application for the GoE funded Ph.D. position – DFT calculations on NRR"**. 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.

Relevant references:

1. “Calculations of product selectivity in electrochemical CO_2 reduction”
   J. Hussain, H. Jónsson & E. Skúlason
   ACS Catalysis, **8** (2018) 5240

2. "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 & J.K. Nørskov,
   Journal of Physical Chemistry C **114** (2010) 18182.

3. "A theoretical evaluation of possible transition metal electro-catalyst for N_2 reduction",
   E. Skúlason, T. Bligaard, S. Gudmundsdóttir, F. Studt, J. Rossmeisl, F. Abild-Pedersen, T. Vegge, H. Jónsson & J.K. Nørskov,
   Physical Chemistry Chemical Physics, **14** (2012) 1235

4. "Electroreduction of N_2 to ammonia at ambient conditions on mononitrides of Zr, Nb, Cr, and V – A DFT guide for experiments",
   Y. Abghoui, A.L. Garden, J. Howalt, T. Vegge & E. Skúlason,
   ACS Catalysis, **6** (2016) 635

5. “Computational screening of rutile oxides for electrochemical ammonia formation”
   Á.B. Höskuldsson, Y. Abghoui, A.B. Gunnarsdóttir & E. Skúlason
   ACS Sustainable Chemistry & Engineering, **5** (2017) 10327

6. “Atomic scale simulations of heterogeneous electrocatalysis: recent advances”
   E. Skúlason & H. Jónsson
   Advances in Physics: X, ***2*** (2017) 481