

Ph.D. and post-doc positions at University of Iceland on experimental electrochemical N₂ reduction reaction

Fully funded Ph.D. scholarship and Postdoctoral fellow positions at the University of Iceland for 3 years supervised by Dr. Egill Skúlason, Professor of Chemical Engineering and Dr. Helga Dögg Flosadóttir, CEO of Atmonia. These positions are available in experimental electrochemical catalysis 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 experimental testing of catalysts suggested from theoretical simulations.

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 for the Ph.D. position. For the post-doc position, only candidates with experience in problem solving and experimental method development as well as track-record of papers on experiments in the field of electro-catalysis in peer-reviewed journals will be considered. For both positions, besides a strong scientific background it is important that the candidates have a good technical writing ability and verbal communication skills.

The project involves electrochemical experiments of N₂ reduction reaction (NRR) on transition metals, metal nitrides, metal oxides, metal oxynitrides and metal sulfides surfaces (thin films and nano-particles) that have been suggested from theoretical screening studies (*see relevant publications below*). Close comparison is made with the theoretical calculations each time and the ultimate goal is to identify new and/or improved catalysts.

Applications should be sent to egillsk@hi.is before **10th of April 2019** with the subject: "**Application for the GoE funded Ph.D. position – Experimental NRR**" or "**Application for the GoE funded post-doc position – Experimental NRR**". The application should include a CV, publication list, 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., M.Sc. and/or Ph.D. research project and are willing to provide a letter of recommendation.

Relevant references:

1. "Calculations of product selectivity in electrochemical CO₂ 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 N₂ 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 N₂ 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