Ph.D. position at the University of Iceland on DFT calculations of electrochemical N_2 oxidation to nitrate

Fully funded Ph.D. scholarship for 3 years from the University of Iceland (UI) has been awarded for the project "*Direct electrochemical nitrogen oxidation to nitrate through rational catalyst design*" supervised by Dr. Egill Skúlason, Professor of Chemical Engineering at the UI. The project will be done in collaboration with Dr. Andrew J. Medford, Assistant Professor at Georgia Institute of Technology, USA.

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 *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 electrochemical N_2 oxidation, where catalysts will be screened for this reaction. Two novel methodologies will be used to model the electro-catalysis: i) The thermochemical model using the computational hydrogen electrode [1] which has been used with great success for other processes such as water oxidation, N_2 reduction and CO_2 reduction [2,3,4]. ii) The electrochemical solid-liquid interface (ESLI) model which is a detailed model setting up a charged interface where charge transfer energy barriers can be calculated as a function of explicitly applied potentials such as has been done previously for the hydrogen evolution/oxidation reactions and the CO_2 reduction reaction [5,6]. The aim of the project is to search for a catalyst that can directly oxidize N_2 to nitrate in an electrochemical cell. However, in both industry and also in nature (enzymes in bacteria) the N_2 molecule is first reduced to ammonia which is then oxidized to nitrate. Therefore, designing a process that can oxidize N_2 directly to nitrate would be a major breakthrough and the predictions would be tested experimentally in our lab.

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 July 2019** with the subject: **"Application for a Ph.D. position at UI – DFT calculations on NOR"**. 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.

References:

1. "Origin of the overpotential for oxygen reduction at a fuel-cell cathode"
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   Journal of Physical Chemistry B, **108** (2004), 17886.

2. “Electrolysis of water on oxide surfaces”
   J. Rossmeisl, Z.-W. Qu, H. Zhu, G.-J. Kroes & J.K. Nørskov,
   Journal of Electroanalytical Chemistry, **607** (2007) 83.

3. “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.

4. “Trends of electrochemical CO2 reduction reaction on transition metal oxide catalysts”
   E. Tayyebi, J. Hussain, Y. Abghoui & E. Skúlason,
   Journal of Physical Chemistry C, **122** (2018) 10078.

5. “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.

6. “Calculations of product selectivity in electrochemical CO2 reduction”
   J. Hussain, H. Jónsson & E. Skúlason,
   *ACS Cata*lysis, **8** (2018) 5240.