Ph.D. position at University of Iceland on DNN+DFT calculations of electrochemical N_2 reduction reaction

Fully funded Ph.D. scholarship at the University of Iceland for 3 years supervised by Dr. Egill Skúlason, Professor of Chemical Engineering. One Ph.D. position is available in theoretical modelling and is supported through a grant entitled "Integrating AI and DFT for sustainable ammonia synthesis – a high-throughput screening study" funded by the Icelandic Research Fund (grant no. 2410761-051). The consortium behind this project are University of Iceland and Fujitsu Limited in Japan. A close collaboration and discussion with the startup company Atmonia ehf. in Iceland is maintained.

The project involves using a combination of AI, deep neural networks (DNN) and DFT simulations to accelerate the search for suitable catalysts for ammonia synthesis. This project will be a frontrunner in the field of theoretical catalysis. Developing sustainable methods for ammonia synthesis is important to combat rising global carbon emissions. An alluring possibility is the electrochemical reduction of nitrogen in an aqueous electrolyte, driven by renewable energy. However, a suitable catalyst has yet to be identified, with a vast composition space of potential catalysts awaiting exploration. In this project, we conduct high-throughput simulations of the catalyst viability of eight classes of transition metal-based materials for ammonia synthesis. The initial screening, which includes strict thermodynamics-based criteria, is performed using a combination of DFT and DNN. Then, a second round of screening is conducted with DFT, probing the stability of the materials identified as promising in the first round. The remaining materials are then proposed as viable catalysts for experimental testing. Additionally, we use a state-of-the-art causal discovery AI to screen the whole dataset generated in the screening study to search for hidden descriptors that, if identified, could be used to facilitate future screening studies.

We are seeking exceptionally qualified applicants for this position. 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 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. Knowledge and skills within DNN simulations is beneficial. 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 **17th of February 2024** with the email subject title: **"Application for Ph.D. position in DNN+DFT simulation for NRR in Feb 2024"**. (Note: If this subject title is not used the application is not considered). 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:

"High-throughput computational screening of doped transition metal oxides as catalysts for nitrogen reduction", Á.B. Höskuldsson, T. Dang, Y. Sakai, A. Ishikawa & E. Skúlason, *Cell Reports Physical Science.* **4**, (2023) 101595

"Self-Supervised Learning with Atom Replacement for Catalyst Energy Prediction by Graph Neural Networks", Y. Sakai, T. Dang, S. Fukuta, K. Shirahata, A. Ishikawa, A. Inoue, H. Kawaguchi, Á.B. Höskuldsson & E. Skúlason
Procedia Computer Science **222**, (2023) 458