Alchemical Perturbation DFT Simulations of High Entropy Alloys for Electrochemical Energy Applications

For: MSc or PhD Students; 12 months

Program supported: Materials for Clean Fuels

Academic Collaborator	NRC Principal Investigator	Associated NRC Research Centre
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Project Description:

High-entropy alloys (HEAs) are a novel, underexplored class of materials consisting of at least five or more elements, and show exceptional properties over conventional alloys. Recently, their remarkable catalytic performance has been shown for CO2 reduction reaction (CO2RR), oxygen reduction reaction (ORR), and hydrogen evolution reaction (HER). Conventional first-principle simulations can explore active and stable electrocatalysts, but due to the large number of possible arrangements of surface sites make this complex and unfeasible for HEAs.

This project aims to substantially expedite the prediction of HEAs catalytic performance by using Alchemical derivatives approach (computational alchemy) to model many facet and composition of HEAs. Alchemical derivatives, which correspond to the change in the energy with respect to changes in the nuclear charge distribution, opens up a promising approach for estimating energy differences between the alloys. The key advantage of a computational alchemy is that no additional information is needed besides a single DFT calculation for binding energy (BE) calculation, and thereafter, large numbers of adsorbate BEs for hypothetical surface structures can be obtained at the minimal computational cost than the conventional DFT methods. These estimates could be used for inverse design of electrocatalysts with only a few calculations to predict a large number of BEs and structure properties of HEAs.

The project will focus on development and implementation of alchemical derivatives to predict volcano plots and catalytic descriptors to identify new high performance HEA's electroctalaysts for CO2RR, OER and nitrogen reduction reactions (NRR) applications. Development of this novel powerful tool is essential for exploring electrochemical performance metrics and discovery of new electroctalaysts. This project is well aligned with the objectives of Materials for Clean Fuel Challenge program (MCF).

Student Profile:

We look for a highly motivated student with a background in computational material or chemistry (or similar disciplines). The chosen candidate will develop and implement alchemical derivatives for HEAs.

As the successful candidate, you will have:

- Prior experience with computer simulations and a strong background in computational materials sciences
- Experience in Density Functional Theory simulations in VASP (Quantum ESPRESSO is a plus)
- Experience of machine learning tools is an advantage
- Skills in programming languages (Python) and Linux
- Basic knowledge of parallel computing will be an asset
- Strong time management skills and the ability to work independently and collaboratively