A Computational Framework Enabled Rational Design of Novel Electrocatalysts/Super Protonic Electrolyte Materials for High Temperature Electrolysis (HTE)

DMREF/HydroGEN EMN Postdoctoral Position

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Hydrogen production via water electrolysis using solid oxide electrolysis cells (SOECs) at elevated temperatures has attracted considerable attention because of its favorable thermodynamics, kinetics, as well as high cost-scaling factor. It is thus considered the most efficient and low-cost option when distributed/small scale hydrogen generation is required, especially from renewables. SOEC systems appear poised for commercialization, but widespread market penetration will require continuous innovation of materials to enhance system lifetime and reduce cost. These novel materials are required to possess unique compositions, structures, morphologies, and architectures that promote the fast transport of ionic and electronic defects, facilitate rapid surface electrochemical reactions, and enhance the tolerance to contaminants at intermediate temperatures. However, the creation of such materials highly rely on empirical and chemical/physical intuition and/or time-consuming trial-and-error experimental efforts in the past due to lack of mechanisms of many charge and mass transport processes associated with operation.

The proposed computational framework is well aligned with the missions of the Designing Materials to Revolutionize and Engineer our Future (DMREF) and Materials Genome Initiative (MGI) programs. Specifically, it is focused on development of novel electrocatalyst towards water oxidation reaction, and optimization of super protonic perovskite electrolyte materials in SOECs under service conditions (e.g., high steam concentration, high current density, etc.), by first-principles density functional theory (DFT) and continuum modeling. The framework will provide the insight for rational design of materials, interfaces, and morphology by addressing the basic science needs for this specific application. It will provide solid support to INL's Node Capability under the HydroGEN Energy Materials Network (EMN), (https://www.h2awsm.org/capabilities/advanced-electrode-and-solid-electrolyte-materials-elevated-temperature-water), greatly accelerating the innovation of the novel materials and resulting performance enhancement and cost reduction in SOECs.

This position requires knowledge and experience in DFT, especially for metal and oxides. Specifically, the postdoc will perform but not be limited to the following work:

- Dissociation-energy assisted catalyst design. The Sabatier principle and volcano plot approaches will be used to guide catalyst design, in which the dissociation energy plays a key role in catalysis towards water oxidation and oxygen evolution reactions.
- *Ab initio* modeling of proton conducting electrolytes. This requires the postdoc to use DFT to calculate the energetics of polaron formation and migration in barium zirconate/cerate system. Furthermore, he/she needs to use continuum modeling to calculate the spatial distribution of oxygen potential inside the SOEC, which is expected to be highly non-linear, given the strong

dependence of electronic conductivity on the oxygen potential, and estimate the electronic transference numbers as a function of temperature, current density, and overpotential.

Familiarity with heterogeneous catalysis is a plus. The expectation for the successful candidate is that the person will be highly motivated and a self-starter, but also be capable of working well and efficiently in a highly team oriented environment.