Accelerating Materials Discovery and Research of Water Splitting Materials through Experimental and Computational Tools and Databases

DMREF/HydroGEN EMN Postdoctoral Position

Lawrence Berkeley National Laboratory (LBNL)

LBNL Principal Investigators: Drs. Francesca Toma, Ethan Crumlin, Adam Weber, Ahmet Kusoglu, Mike Tucker, Jason Cooper, and Nemanja Danilovic

We propose multiple projects complementary to the goals of the Designing Materials to Revolutionize and Engineer our Future (DMREF) and the Materials Genome Initiative (MGI) programs using existing HydroGEN Energy Materials Network (EMN) capability nodes. The experimental and modeling capabilities listed below help inform the computational machinery necessary for large-scale materials selection as applied to water-splitting technologies, in particular, low- and high-temperature electrolysis (LTE, HTE) and photoelectrochemical (PEC) water splitting. The goals of the DMREF/EMN postdoctoral scholars would be to utilize one or more existing capability nodes, or to develop the necessary experimental capability within a node to:

1. Characterize intrinsic materials properties related to their activity, selectivity or stability of electrocatalytic, or photovoltaic water-splitting materials (PEC, LTE, HTE) that are required to build computational models of the devices these materials would go into.
2. Characterize materials properties and emergent phenomena due to integration of multifunctional components from tests beds and prototype devices in order to produce key parameters required for multiphysics, multiscale models of devices.
3. This includes development of and enhancement of novel characterization techniques in order to extract the necessary intrinsic materials properties or materials properties from device level operation or in situ conditions.
4. Provide data to the EMN data hub and interact with EMN data scientists to help integrate the data hub with other materials property databases, thereby building a nascent large-scale materials selection data repository and search engine.

Relevant LBL Capability Nodes

Intrinsic materials selection and properties

1. In-situ and operando nanoscale characterization capabilities for photoelectrochemical materials and integrated assemblies (PEC)
2. Ionomer characterization and understanding (LTE, PEC)
3. Photoelectrochemical device in situ and operando testing using X-rays (HTE, LTE, PEC)
4. Scanning droplet cell for high throughput electrochemical evaluation (LTE, PEC)
5. Photophysical characterization of photoelectrochemical materials and assemblies (PEC, LTE)
6. Probing and mitigating chemical and photoelectrochemical corrosion of electrochemical and photoelectrochemical assemblies (PEC, LTE, HTE)

Multiscale test beds materials selection and properties

1. Multiscale modeling of water-splitting devices (LTE, PEC, HTE)
2. Metal supported solid oxide cells (HTE)
3. Water splitting device testing (LTE, PEC)
4. Outdoor testing facility for solar water splitting devices (PEC)

Capability development and enhancement opportunities

1. Probing and mitigating chemical and photoelectrochemical corrosion of electrochemical and photoelectrochemical assemblies (PEC, LTE, HTE)
    a. Develop in situ technique to probe materials degradation during electrochemical operation. Develop trend in activity and stability for electrochemical and photoelectrochemical materials.
2. Photoelectrochemical device in situ and operando testing using X-rays at the Advanced Light Source (HTE, LTE, PEC)
    a. Link materials activity and stability in situ and operando using X-rays.
3. Ionomer characterization and understanding (LTE, PEC)
    a. Link polymer properties to their structure under constrained and unconstrained conditions as a function of molecular weight, side chain size, and polymer chemistry.