JCAP Tools

The Joint Center for Artificial Photosynthesis (JCAP), established by the U.S. Department of Energy in 2010 as the Fuels from Sunlight Energy Innovation Hub, aims to advance the science needed to convert sunlight, water and carbon dioxide into a range of commercially useful fuels. JCAP has developed numerous tools and methods to address its scientific goals, many of which have broad applicability in the field of artificial photosynthesis. This document presents a subset of these capabilities; JCAP's publications [https://solarfuelshub.org/publications] provide more detailed information.

Benchmarking

JCAP has developed standardized measurement protocols for half and full-cell reactions pertinent to solar fuel generation. Standard instrumentation, protocols for its operation, and best practices for reporting and visualizing the resulting data have been detailed in several papers. These methods have been applied to establish an extensive database of benchmarked thin film[1] and nanoparticulate[2] electrocatalysts for water oxidation and hydrogen generation. JCAP has also focused on developing standardized cells and analytical methods for quantification of CO_2 reduction products, with the cell designs and methods[3] published for use by the community. These developments are intended to allow researchers to compare the performance of one catalyst to another within a lab and between labs in a consistent and quantitative manner.

In situ and operando capabilities

JCAP researchers have expanded methods for laboratory- and synchrotron-based *in situ* and *operando* studies of electrocatalysis. The synchrotron work has involved partnerships with the Advanced Light Source at Lawrence Berkeley National Laboratory and the Stanford Synchrotron Radiation Lightsource at SLAC National Accelerator Laboratory. New synchrotron techniques include real-time studies of transformations and electronic characteristics[4] of electrolyte-electrocatalyst interfaces by X-ray photoemission spectroscopy, and electrocatalyst structure while in contact with electrolyte[5] or humidified vapor[6] by grazing incidence X-ray scattering. Each of these techniques is now available to the user community. Laboratory studies[7] coupling multiple surface-sensitive electrochemical techniques provide complementary molecular-level information.

High-throughput experimentation and theory pipeline for materials discovery

JCAP has established and deployed a high-throughput facility that uses a coordinated pipeline for the discovery of new light absorbers, photocatalysts, and electrocatalysts using combinatorial techniques. Experiment and theory[8] are tightly integrated to identify functional solar fuels materials in broad materials search spaces. Rapid characterization using high performance scanning instruments such as the scanning droplet cell[9] and online mass spectrometry[10] allow materials and interfaces[11] with desired properties to be identified then synthesized on a larger scale for in-depth study. An extensive Materials Experiment and Analysis Database (MEAD) [https://www.htejcap.org/hte_jcap_app/document/search] and associated data science techniques[12] have resulted from the work, and are available to the materials community.

Testbeds and Prototyping

JCAP researchers have created new concepts for solar fuels generator systems and accompanying multiphysics models. The systems provide platforms that allow fundamental efficiencies and chemistries to be determined for new catalysts and light absorbers, and enable testing of durability over time under well-controlled conditions. The models enable architectural and component characteristics and phenomena that affect efficiency and performance to be identified and explored. Publications describe solar water splitting devices[13] and CO_2 reduction systems[14] using liquid electrolytes. JCAP has also focused on vapor-fed systems[15] and membrane-electrode assemblies[16] that confer a number of advantages for efficiency and durability. Publications describe both dark electrolysis systems that could be coupled to external photovoltaics,[17] and fully integrated, photo-driven vapor fed assemblies.[18]

Theoretical methods for electrochemical systems

Code packages and computational techniques developed by JCAP's theory researchers have been used extensively in the Hub's science programs. They have been placed in open source or open access for use by the community. Information on their design and applications can be found in publications. They include

- A formalism for calculating Pourbaix energetics[19] [http://materialsproject.org]
- An amorphous solid phase structure generator[20] [https://bitbucket.org/zhfan_dertba/bond-switching]
- NA-MD: code for nonadiabatic molecular dynamic simulation, implementing a special matrix algorithm for carrier relaxation.[21] [https://bitbucket.org/zhfan_dertba/namd_basic/]
- entos: A suite of electronic structure and dynamics tools using quantum embedding and machine learning methods[22] [www.entos.info]
- PERTURBO: code for calculating electronic excitation and dynamics in solids [http://perturbo.caltech.edu/]
- JDFTx: grand canonical quantum mechanics using constant potential for electrochemical systems[23] [http://jdftx.org [*SoftwareX* **6**, 278 (2017)]
- RexPoN: reactive force fields for very accurate multiscale simulations[24] [https://github.com/login]
- PQEq: dynamic charge distribution and polarization for use in force fields for large scale MD simulations[25] [https://github.com/login]

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