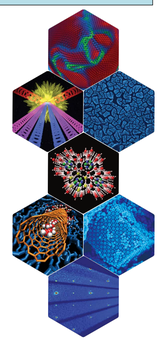
Fundamental Research Underpinning Hydrogen and Fuel Cells
Office of Basic Energy Sciences
U.S. Department of Energy

U.S. DEPARTMENT OF ENERGY | Office of Science

Basic Energy Sciences (BES)

Mission

To understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels.



BES fulfills its mission through:

Supporting **basic research** to discover new materials and design new chemical processes that underpin a broad range of energy technologies.

Operating **world-class scientific user facilities** in X-ray, neutron, and electron beam scattering as well as in nanoscale research.

Managing **construction and upgrade projects** to maintain world-leading scientific user facilities.

Organization

Office of Basic Energy Sciences
Harriet Kung, Director

Materials Sciences and Engineering Division	Scientific User Facilities Division	Chemical Sciences, Geosciences, and Biosciences Division
Linda Horton, Director	James Murphy, Director	Bruce Garrett, Director

Funding Motifs

Increasing scope and size

- Core Research (>1,000 projects, ~$500M/year)
  Single investigators ($150K/year) and small groups ($500K-$2M/year) engage in fundamental research related to any of the BES core research activities. Investigators propose topics of their choosing. Includes awardees under the SC Early Career Research Program.
- Energy Frontier Research Centers ($110M/year)
  $2-4 million/year research centers for 4-year award terms; focus on fundamental research described in the Basic Research Needs Workshop reports.
- Computational Chemical and Materials Sciences ($25M/year)
  - Up to $2-4 million/year research centers for 4-year award terms; focus on delivering open source, experimentally validated software and the associated data for predictive materials and chemical sciences in preparation for exascale computing.
- Energy Innovation Hubs ($38M/year)
  Research centers, established in 2010 ($15-25 million/year), engage in basic and applied research, including technology development, on a high-priority topic in energy that is specified in detail in an funding opportunity announcement (FOA). Project goals, milestones, and management structure are a significant part of the proposed Hub plan.

User Facilities

Access available **at no cost** for non-proprietary research, through a merit based peer review of brief proposals.

Strategic Planning

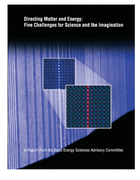
BES reports, workshops, and roundtables seek to **encourage transformative, basic science breakthroughs** by tapping the creative imagination of the research community.

Recent Basic Research Needs (BRNs) Workshops

Catalysis Science

Instrumentation

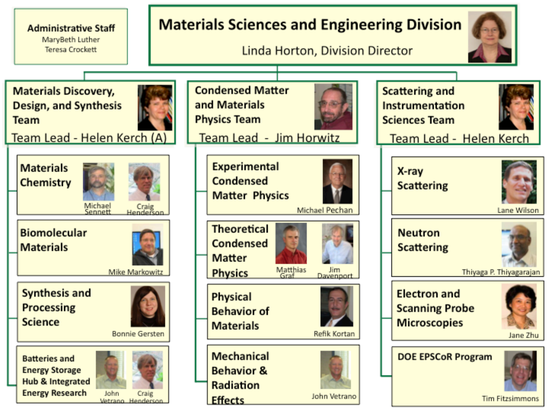
Grand Challenge Reports



2007

2015

BES Research is Grouped by Scientific Topic



- As with all technology areas, there is no Hydrogen and Fuel Cell-specific Funding Opportunity Announcements in FY 2018 though it is one of the topics in the current Energy Frontier Research Center solicitation
- BES funding for fundamental research underpinning fuel cells and hydrogen has remained steady between $20,000k and $25,000k for the past several years.
- Research topics include hydrogen storage, nanoscale catalysts, membranes/separations, bio-inspired hydrogen production and solar hydrogen production
- Annual solicitations applicable for basic research in these areas are our "open" core FOA and our Early Career Research Program. The Energy Frontier Research Center Program supports research in these areas as well.
- BES coordinates with other DOE Offices through the internal working group, and with other Government Agencies through participation in the Interagency Working Group
- Recent Basic Research Needs workshop on Catalysis Science was held in 2017 and the report is available on the BES web site

Highlights of BES-Funded Basic Research

Introducing Chemical Functionalities into the Nano Space

Scientific Achievement

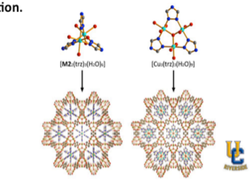
New functional materials have been synthesized using metal-organic clusters as pore-partitioning agent inside nanoporous channels.

Significance and Impact

With diverse and unprecedented compositions and functionalities, both on the framework and within the channel, these new materials have a number of potential applications such as catalysis, fuel storage, and chemical separation.

Research Details

- By matching distribution symmetry of open-metal site on the framework with organic-metal clusters within the channel, the pore space is partitioned and functionalized, resulting in a huge family of multi-functional heterometallic materials.
- The rich chemical compositions and functionalities including catalytic open-metal sites within the nanopore space open up new possibilities for selective gas storage, separation, and catalysis.

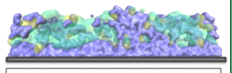


X. Zhao, P. Feng, et al. J. Am. Chem. Soc. 2016, 138, 15102-15105.
Q. Zhai, P. Feng, et al. Acc. Chem. Res. 2017, 50, 407-417.
Q. Zhai, P. Feng, et al. Nature Communications, DOI: 10.1038/ncomms13645.

Proton Solvation and Transport in Complex Materials and Acidic Solutions

Scientific Achievement

In systems involving interfaces between catalytic surfaces and proton exchange membranes, reactive molecular dynamics (RMD), at least 1000 times faster than *ab initio* MD, has shown how the hydrophilicity of the surface affects the membrane structure, water network formation, and proton transport



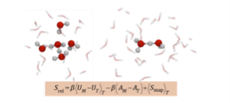
Thin film PEM showing water regions in blue, polymer regions in green, and substrate in black.

Significance and Impact

Hydrophilic surfaces were found to promote robust water layer formation at the interface. Additionally, decreasing interaction between charged sulfonate groups and hydronium molecules increasing diffusion

Research Involved

- All-atom RMD simulations compared the effects of surface hydrophilicity, membrane morphology, and temperature on structure and proton diffusion
- A novel RMD model was developed using a relative entropy minimization (REM) scheme and data from *ab initio* molecular dynamics (AIMD)
- A spectroscopic model coupling RMD with electronic structure calculations was developed to improve the understanding and interpretation of acid vibrational spectra



Snapshots of Eigen ($H_9O_4^+$) and Zundel ($H_5O_2^+$) cations from AIMD simulations used in RMD methodology.

Biswas, R.; Carpenter, W.; Fournier, J. A.; Voth, G. A.; Tokmakoff, A., *J. Chem. Phys.* **2017**, *146*, 154507.

THE UNIVERSITY OF CHICAGO | James Franck INSTITUTE

Putting the Cap on – Trapping Gases in Metal Organic Frameworks

Scientific Achievement

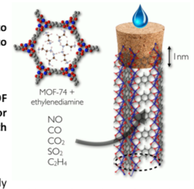
Post-exposure of metal organic framework (MOF) materials to ethylenediamine (EDA) forms a monolayer cap, which allows us to trap small molecules, even when they are only weakly bound.

Significance and Impact

The ability to create a molecular surface barrier layer on MOF external surfaces constitutes an entirely new paradigm for trapping weakly adsorbing molecules within MOFs, with importance for gas storage and sequestration applications.

Research Details

- Molecules such as NO, CO, CO_2, SO_2, and C_2H_4 were successfully retained in two prototypical materials MOF-74 and HKUST-1, as confirmed by *in-situ* IR spectroscopy.
- Water molecules were shown to easily penetrate this molecular EDA barrier layer and displace previously trapped gases, constituting an easy release mechanism.
- The capping mechanism and the "gate opening" disruption of the H-bonded amine groups of EDA by water molecules were fully explained by *ab initio* modeling.



Scheme of trapping molecules in MOF-74 by post-loaded EDA. X-ray photoelectron spectroscopy combined with gas-cluster ion sputtering and low energy ion spectroscopy measurements establish that EDA is only adsorbed as a monolayer on the exterior surface of MOF crystals (< 1nm thick), thereby acting as capping layer.

K. Tan et al., Nat. Commun. 7, 13871 (2016)

Work was performed at UTD, Wake Forest, and Rutgers.

UTD | Wake Forest University | Rutgers

Combining Theory and Experiment in Electrocatalysis: Insights into Electrocatalyst Design

Scientific Achievement

Reviews state-of-the-art developments and remaining challenges in the design of active and selective electrocatalysts for a number of energy conversion processes.

Significance and Impact

The combination of theory and experiment provides insight into materials design for electrocatalysts, uncovering broader governing principles that can guide catalyst development more generally.

Research Details

- A descriptor-based approach can rationalize catalyst performance; a key starting point in design.
- Underlying limitations on catalyst performance are identified, often attributed to unfavorable scaling relations, providing guidance to experimental approaches to overcome them.
- These material design concepts are described in detail for reactions involving hydrogen and oxygen, and can be extended to emerging clean energy reactions such as hydrogen peroxide production, carbon dioxide reduction and nitrogen reduction.

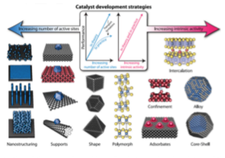
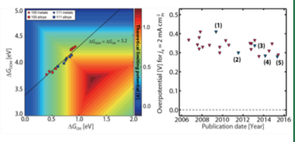


Illustration of the way unfavorable scaling between key descriptors of the oxygen reduction reaction leads to an "overpotential wall" in terms of (best) reported experimental overpotentials over the last ten years.



Z. W. Seh, J. Kibsgaard, C. F. Dickens, I. Chorkendorff, J. K. Nørskov, T. F. Jaramillo, *Science* (2017) DOI: 10.1126/science.aad4998

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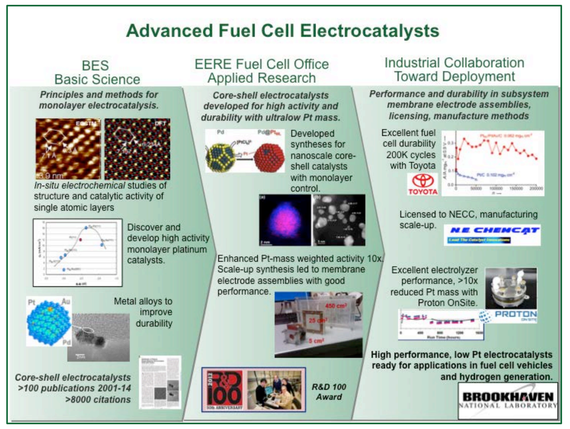
Science to Technology



BES Funding Opportunities

General Core Proposal Information

Annual Funding Opportunity Announcement (FOA):
http://science.energy.gov/grants/foas/open/

Contact the program manager for the program of interest to discuss your idea (**email** is usually best).

Consider submitting a **pre-application** (or white paper) to the DOE program (2-3 pages)

- The process for submitting the white paper can vary by CSGB program, so contact the program manager prior to submission.
- Pre-applications are evaluated internally for appropriateness and with regard to program scope and needs
- Encourage/Discourage decision is communicated to the PI

Early Career Research Program (since FY10)

- 5-year awards, $150,000/yr for University researchers
- **Eligibility:** Within 10 years of receiving a Ph.D., either untenured assistant or associate professors on the tenure track

Tips

1. Familiarize yourself with what types of projects are funded in CSGB and what program(s) fit your proposed work.
2. Contact the program manager of the relevant program before submission with any questions.
3. Adhere to all guidelines in the Funding Opportunity Announcement.

Workforce Development for Teachers and Scientists (WDTS)

Office of Science Graduate Student Research (SCGSR) Program
3-12 month supplemental support to conduct research at a DOE laboratory

Science Undergraduate Laboratory Interns (SULI) Program
Supports ~750 undergraduates at one of 17 DOE labs or facilities

Summer School Programs
Nuclear Chemistry, Applied Geophysics, and Particle Accelerator Schools

Important Links and Resources

General Links

BES: http://science.energy.gov/bes
Early Career: http://science.energy.gov/early-career/
User Facilities: http://science.energy.gov/bes/suf/user-facilities
WDTS: http://science.energy.gov/wdts

Resources

Funding Opportunity Announcement (FOAs):
http://science.energy.gov/grants/foas/open/
Reports: http://science.energy.gov/bes/community-resources/reports/
PAMS (grant management system):
http://pamspublic.science.energy.gov/