EFRC: ENERGY FRONTIER RESEARCH IN EXTREME ENVIRONMENTS (EFREE)

UPDATED: AUGUST 2016

AWARDS: $15.0M (August 2009 – July 2014); $10.0M (August 2014 – July 2018)	
WEBSITES: http://science.energy.gov/bes/efrc/centers/efree/; https://efree.carnegiescience.edu	
TEAM: **Carnegie Institution (Lead):** Russell Hemley (Director), Timothy Strobel, Stephen Gramsch, Reinhard Boehler, Maria Baldini; **California Institute of Technology**: Brent Fultz; **Colorado School of Mines**: P. Craig Taylor, Lakshmi Krishna; **Cornell University**: Roald Hoffmann, Neil Ashcroft; **George Washington University:** Tianshu Li, Russell Hemley; **Lehigh University:** Kai Landskron; **Pennsylvania State University:** John Badding, Vincent Crespi, Nasim Alem; **University of Tennessee**: Konstantin Lokshin	

SCIENTIFIC MISSION AND APPROACH

The mission of EFree is to accelerate the discovery and synthesis of new energy materials using extreme conditions. While most materials are created at or near ambient conditions, exploiting extreme environments, notably high pressures and temperatures, has tremendous potential for manipulating matter to synthesize next-generation materials with transformative impacts on energy. Moreover, extreme environments are capable of producing materials with unprecedented mechanical, thermal, and electronic properties. The Center's research projects are organized around three Energy Focus Areas:

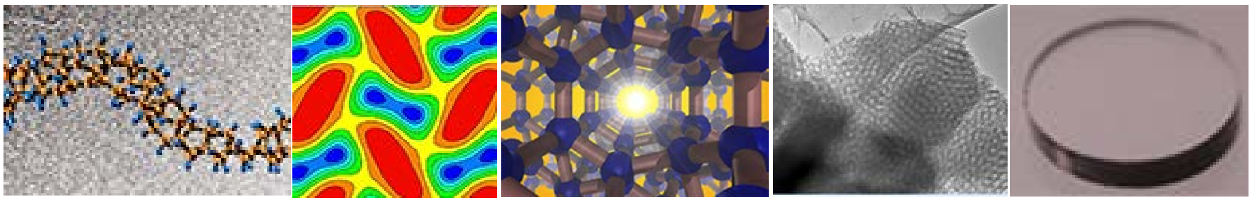
1) **Advanced Structural Materials**: Use of extreme environments to develop tailored synthetic routes for the discovery, characterization, and preparation of new classes of energy materials such as new nanophase carbons and porous materials

2) **Novel Energy Conversion Materials**: Use of extreme environments to create new energy conversion materials and recover them to ambient conditions for enhanced solar energy uptake and other energy conversion applications.

3) **Revolutionary Energy Transport Materials:** Use extreme environments to understand the fundamental physics of electron transport in materials, and optimize structure and composition to create new materials with enhanced electrical transport such as high T_c superconductivity.

SELECTED SCIENTIFIC ACCOMPLISHMENTS

- Carbon nanothreads - a new allotrope of nanocrystalline carbon - was discovered, characterized, and recovered to ambient conditions. The material has chemical bonding properties identical to that of diamond and is considered an ultrastrong, lightweight material with numerous applications.
- A new allotrope of silicon, Si_{24}, having an open-framework structure was developed using a high-pressure precursor method. The material has been recovered at ambient conditions and possesses a quasi-direct band gap making it a potentially highly efficient photovoltaic.
- Porous structures based on dense SiO_2 frameworks were synthesized using a novel high-pressure nanocasting method. The material has accessible mesopores and a wide pore size distribution.
- Metallization and superconductivity was discovered at high pressure in $BaReH_9$, the most hydrogen-rich ionic salt. The result provides key information needed to understand the superconducting properties expected for hydrogen and other hydrogen-rich materials.
- Advanced theoretical calculations predicted the structures, stability, and physical properties of new classes of light element, very high T_c superconductors, including new hydride phases and analog carbon-based superconductors predicted to be stable under ambient pressure.



EFree research, from left: Structure of a one-dimensional carbon nanothread. Electron density map of crystalline dense Li showing an inverse relationship to that of hydrogen. Structure of Si_{24}, showing the open framework structure. TEM image of highly crystalline mesoporous stishovite synthesized using high-pressure nanocasting. Single-crystal diamond window grown by CVD techniques.

IMPACT

- Developments in high-pressure cell designs have enabled neutron diffraction to 100 GPa at the Spallation Neutron Source (SNS). The partnership between EFree and the SNS is yielding advances in both technique development and fundamental science at several neutron scattering beamlines.
- The paper reporting the discovery of carbon nanothreads is in the ISI top 1% for materials science and has been highlighted in many popular scientific publications, newspapers and broadcast news organizations. These materials promise outstanding properties related to their unique high-strength bonding geometry.
- A US patent has been awarded for the development of zeolite-templated carbon (ZTC), a nanostructured material that promotes interactions between molecules physisorbed on its surface at high pressure. ZTC greatly improves physisorption of gases such as CH_4, C_2H_6, Kr and CO_2.
- The paper reporting the synthesis of Si_{24} was the most highly rated paper in *Nature Materials* for papers of similar age, and in the 99th percentile of all papers tracked, as of August 2016. A US patent is pending for the synthesis and several inquiries concerning capital investment have been received.
- Recent advances in CVD diamond growth methods have been put into production at **Washington Diamonds Corporation,** http://www.wdlabgrowndiamonds.com. Continued interactions are helping to optimize the growth of material for scientific and technological applications.

PUBLICATIONS AND INTELLECTUAL PROPERTY

As of May 2016, EFree had published 285 peer-reviewed publications cited over 4,500 times and filed two US patent applications and one foreign patent application. One patent has been issued. The following is a selection of impactful papers:

- Fitzgibbons, T. C., Guthrie, M., Xu, E. S., Crespi, V. H., Davidowski, S. K., Cody, G. D., Alem, N. & Badding, J. V. Benzene-derived carbon nanothreads. *Nature Mater.* **14**, 43-47, doi: 10.1038/NMAT4088 (2015). [**43 citations**]
- Kim, D. Y., Stefanoski, S., Kurakevych, O. O. & Strobel, T. A. Synthesis of an open-framework allotrope of silicon, *Nature Mat.* **14**, 169-173, doi: 10.1038/NMAT4140 (2015). [**33 citations**]
- Naumov, I., Hemley, R. J., Hoffmann R. & Ashcroft, N. W. Chemical bonding in hydrogen and lithium under pressure*. J. Chem. Phys.* **143**, 064702, doi: 10.1063/1.4928076 (2015). [**4 citations**]
- Boehler, R., Guthrie, M., Molaison, J., dos Santos, A. M., Sinogeikin, S. V., Machida, S., Pradhan, N. & Tulk, C. A. Large-volume diamond cells for neutron diffraction above 90 GPa. *High Press. Res.* **33**, 546-544, doi: 10.1080/08957959.2013.823197 (2013). [**14 citations**]
- Niu, H., Chen, X. Q., Wang, S., Li, D., Mao, W. L. & Li, Y. Families of superhard crystalline carbon allotropes constructed via cold compression of graphite and nanotubes. *Phys. Rev. Lett.* **108**, 135501, doi: 10.1103/PhysRevLett.108.135501 (2012). [**75 citations**]