Center for Energy Frontier Research in Extreme Environments (EFree)
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Mission Statement: *To accelerate the discovery and creation of energy-relevant materials using extreme pressures and temperatures.*

The critical shortage of abundant, affordable, and clean energy calls upon novel materials that are superior to any known material existing today with extreme properties for energy production, storage, conversion, and transfer. The extreme pressure-temperature (*P-T*) environments present a vast, unexplored, fertile ground to search for transformative materials and phenomena. The Center approach is essential for advancing the high-pressure technology and allying the high-pressure community efforts to accelerate breakthroughs in the energy technologies.

High pressure categorically alters physical properties of phonon, electron, and structure and chemical properties of bonding, reactivity, and kinetics. Pressure pushes materials across conventional barriers between insulator and superconductor, fluid and solid, molecular and extended frameworks, and the vigorously reactive and the inert. In the pressure dimension, creation of novel materials and observation of novel phenomena become the rule rather than exception. The extreme *P-T* studies provide a new route towards discovering advanced structural materials and new materials with enhanced performance for energy transformation (*i.e.* solar, mechanical, chemical to electrical), energy storage (*i.e.*, batteries, capacitors, hydrogen), and energy transmission, sensing and monitoring.

EFree organizes a team of the nation's leading scientists with complementary expertise in high-pressure science and technology, theory and experimentation, physics, chemistry, geoscience, and materials science. EFree develops critical technologies at national facilities and the Carnegie Institution, including the next-generation high *P-T* devices and the integration of extreme environments with synchrotron x-ray, neutron, laser, optical, electronic, magnetic, and nano-scale probes. With this enabling platform, the EFree management directs and monitors dozens of research projects aiming for transformational advances in three thrust areas.

1. Novel Chemical Energy Under Extreme P-T – Pressure drastically changes chemical speciation, dissolution, reactivity, combustion, catalysis, absorption, photochemistry, and electrochemistry. Pressure may create dozens of novel phases with very different properties in an average chemical system; many of them may be quenchable and may carry potential applications for energy generation, storage and transportation. The interest in high-pressure hydrogen has recently extended well beyond the elemental forms to encompass hydrogen-containing molecular alloys and compounds for hydrogen storage applications. EFree conducts a broad-based research program that includes work on the elemental states and those with hydrogen in chemical compounds, where results in one area enhance work in the other.

2. Novel Superconducting, Electronics, and Magnetic Materials Under Extreme P-T – Pressure is opening up broad new vistas on superconductivity from simple elements to complex organic and inorganic materials and the creation of new electronic and magnetic materials of great significance to energy science. Pressure strongly effects emergent properties as well as ordinary electro-magnetic materials, including high-temperature superconductivity, topological insulators, charge- and orbital-density waves, electronic phase separation, magneto-capacitance, multi-ferroics, spintronics, Mott insulators, heavy fermions, colossal magneto-resistivity, polar energy materials, and quasi low-dimensional materials,

thus addressing problems ranging from efficient charge injection in photovoltaic devices to lossless electrical transmission over superconducting lines. Pressure-tuning plasmons, excitons, and electron dynamics are providing the fundamental information necessary for the grand challenge of controlling materials processes at the level of electrons.

3. Novel Nanophase, Mesoporous, Amorphous and Structural Energy Materials Under Extreme P-T – EFree addresses the underlying origin of pressure-induced transitions between crystalline and amorphous materials, and the creations of nanoscaled structures and orders. The dimensionality and size-scale of these materials are closely related to their applications in light emission, catalysis, filtering, membranes, etc. and potentially impact energy efficiency, production, utilization, and storage. EFree applies variable high-*P, T,* and strain rate to synthesize new structural materials such as diamond, cBN, and tough lightweight carbon-based materials, and to study their response and resistance under extremely harsh *P-T* and chemical environments.

To recover the novel high-pressure materials metastably at ambient pressure far away from equilibrium is central to the EFree approach. Mounting examples reveal that the combination of high pressures and low temperatures not only *brings* matter, but also *sustains* matter, very far away from equilibrium. In these studies, pressure provides a powerful means for continuously tuning the free energy of the system; x-ray photons excite systems into highly metastable states, and low temperature and chemical tuning prevent the system from reaching equilibrium. By varying these parameters, characterizing the dynamically compressed or stressed and electronically excited materials with time-resolved probes, and combining these efforts with first-principles calculations, transition mechanisms and energy landscapes can be revealed. Such knowledge is essential for the recovery of materials to ambient conditions for use in numerous energy applications.

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