## Near Room Temperature Superconductivity at Extreme Conditions: Centerwide Discoveries at CDAC

*by Eva Zurek (University at Buffalo, State University of New York) and Maddury Somayazulu (HPCAT, X-ray Science Division, Argonne National Laboratory)*

Ever since the observation of superconductivity in mercury below a critical temperature, ($T_c$), of 4.2 K in 1911, scientists have searched for a material whose $T_c$ approaches room temperature. Superconductors are employed in magnetically levitating trains, in strong electromagnets, and in particle accelerators. Moreover, because electricity passes through a superconductor without any resistance, replacing copper wires with superconducting power lines could save a tremendous amount of energy. Unfortunately, the materials that are commercially employed need to be cooled by liquid helium or nitrogen to below their $T_c$ to realize their superconducting properties. Recent breakthroughs at the Capital/DOE Alliance Center (CDAC) may change this state of affairs, leading ultimately to the century-old dream of creating useful materials that superconduct at or near room temperature.

In 1968, Neil Ashcroft predicted that hydrogen in a hypothetical atomic metallic state at very high pressures, would be a conventional (i.e., electron-phonon), high-temperature superconductor. In 2004, he predicted that doping hydrogen with a second element could lower the metallization pressure required but still keep all of the properties conducive to high $T_c$ superconductivity. Since then, the development of computational methods for crystal structure prediction using quantum-mechanical calculations and dramatic increases in supercomputing capabilities has made it possible for researchers to study theoretically the compounds that can be synthesized under high pressure and their properties.

The breakthroughs at CDAC began with the prediction of new classes of superhydride materials that have calculated $T_c$s near room temperature.[1] The work was performed by Hanyu Liu under the direction of Center director Russell Hemley and CDAC research scientist Ivan Naumov. One of the most promising materials, $LaH_{10}$, then was synthesized by the team very close to the predicted pressures of 180 GPa (about half of the pressure in the Earth's core) using diamond anvil cell techniques.[2] These experiments were led by CDAC postdoc (and former Center student at Berkeley) Zachary Geballe at the NNSA-funded HPCAT synchrotron x-ray facility at the Advanced Photon Source. The team then spent a year developing new experimental techniques to both carefully synthesize and measure the superconducting properties by electrical conductivity and magnetic susceptibility at megabar pressures. This work was led by former CDAC research scientists Maddury Somayazulu and Muhetaer Ahart. The team then confirmed in multiple measurements the predicted very high $T_c$ value of 260 K near 200 GPa, which is the current highest temperature superconductor yet found experimentally.[3]

These developments in CDAC have led to a broader Center-wide research initiative involving theory and experiment. In a recent article, CDAC university partner Eva Zurek and her student Tiange Bi, have reviewed the theoretical investigations that have searched for superconductivity in binary hydrides under pressure.[4] The highest $T_c$ values have been predicted for a subset of the alkaline and rare earth polyhydrides, such as $MgH_6$, $LaH_{10}$, $YH_9$, and $YH_{10}$. In these compounds, the hydrogen lattices resemble chemical compounds called clathrates, and these unique structures turn out to be key for the extremely high $T_c$ values. The $LaH_{10}$ crystal structure is composed of face-sharing hydrogenic polyhedra that contain square and hexagonal faces, and the lanthanum atom lies in the center of each polyhedron (see Figure 1). The effort is being extended in CDAC to other areas of 'materials by design'—the new paradigm in materials science—taking advantage of the diverse capabilities and expertise across the Center.

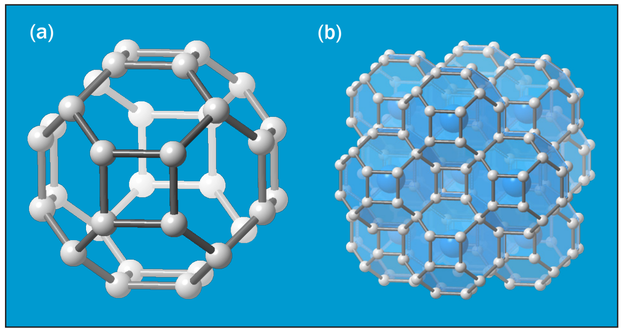


*Figure 1: (left) The hydrogenic clathrate cage that is found within Fm-3m $LaH_{10}$, and (right) its extended crystal structure.*

Researchers worldwide are studying these exciting compounds. The findings of the CDAC scientists were soon confirmed by the theoretical group of Yanming Ma and the experimental group of Mikhail Eremets who, in addition, observed other characteristic signatures of superconductivity. The Meissner effect (the expulsion of a magnetic field by the superconductor) still must be demonstrated, and experiments are underway to verify the theoretical predictions of high-temperature superconductivity in other binary hydrides under pressure. Meanwhile, theoretical groups have started finding related materials that will be very high $T_c$ superconductors at lower pressures and, potentially, even higher temperatures, for example in ternary hydride systems.

### References

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