PSC & (SC)²: Research for Clean Energy

Since the 1999 founding of (SC)², 55 (SC)² research groups, including 114 researchers, have used PSC systems for a range of clean-energy related projects, including designs for advanced power turbines, fluidized-bed combustion, and a reactor to produce power from gasified coal. This work has used more than 6.8 million hours of computing time, over 285,000 hours during the past year.

Pure Hydrogen from Coal Gas

Membranes aren’t only ear drums and cell walls. NETL researchers are developing advanced membrane technologies that can, among other things, separate pure hydrogen from the “syn gas” produced in reactors that convert coal into gases. The high-purity hydrogen that results is a valuable clean-energy commodity — for hydrogen fuel cells and many other industrial uses. The overall goal is to improve the efficiency and robustness of these membranes, conventionally metallic alloys of copper and palladium, so that they can be efficiently integrated into coalconversion processes.

Materials scientist Michael Gao of NETL (and URS Corporation) has used PSC’s Blacklight to accelerate design and development of new, improved membrane alloys of copper-palladium with a third element (ternary alloys) through quantum-mechanical simulations. One project (illustrated by the graph) involves calculating the “enthalpy” — a thermodynamic property — of proposed compounds with different alloying elements.

“We look at the periodic table,” says Gao, “and take atoms to put into virtual alloys. These computations allow us to test hundreds of possibilities and select the most viable candidates to test in the laboratory. We accelerate materials development and shorten the time to improved hydrogen separation performance at reduced cost.” Gao collaborates in these studies with Bryan Morrone’s group in NETL-Pittsburgh, Andrew Gellman’s group at Carnegie Mellon University, and Ömer Doğan’s group in NETL-Albany.