Computational Science Guides and Accelerates Hydrogen Research

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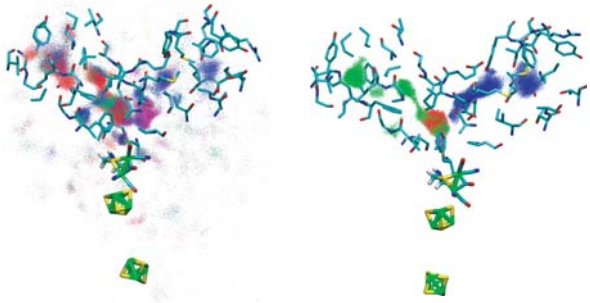
Accomplishment: Through computational science, researchers at NREL have enhanced hydrogen-related research and development in areas such as storage and photobiology (first reported in March 2009).

Context: Computational science uses simulation, numerical analysis, and visualization to advance hydrogen research at NREL. With these tools researchers can examine complex systems and natural phenomena to guide and prioritize research and understand experimental results. Progress is accelerated and costs are reduced.

Computational Science Supports HSCoE Research

Engineered Nanospaces	• Simulated pore size for enhanced physisorption • Established theoretical relationship between volumetric and gravimetric capacity
Doped Materials	• Theorized metal dispersion for boron substituted carbon • Guided enhancement of metal dispersion and hydrogen sorption by boron substitution of graphite
Binding of Dihydrogen	• Determined mechanism and promise on nanoscale • Investigated macroscopic materials
Spillover	• Confirmed feasibility of energetics, thermodynamics, and kinetics

Storage: Achieving high-capacity hydrogen storage at ambient conditions is a challenge that depends on a solid understanding of hydrogen-material interaction. NREL researchers who work with the U.S. Department of Energy (DOE) Hydrogen Sorption Center of Excellence (HSCoE) are using computational science techniques to study these interactions. They have advanced their research in areas that include engineered nanospaces, doped materials, enhanced binding of dihydrogen, and spillover (see table for details).



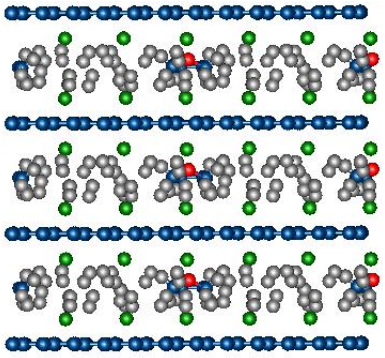
Researchers at NREL used computational modeling to discover pathways for H_2 (Figure A) and O_2 (Figure B)

NREL researchers proposed a group of novel materials such as organometallic buckyballs, metallo-carbohedrene crystal, and intercalated graphite for hydrogen storage. Simulation also revealed the mechanism of hydrogen spillover diffusion in carbon-based materials. The principles of organometallic sorbents not only created a major research focus within the HSCoE but also established a new direction in the broader research community. NREL experimentalists confirmed conceptually the co-intercalation of graphite for hydrogen storage, and they are currently focused on improving the storage properties.

Photobiology: Researchers use computational science to model the structure and function of [FeFe] hydrogenase enzymes for the design of next-generation hydrogen production catalysts. To investigate the biotechnological limitations of [FeFe] hydrogenase enzymes, NREL models protein/protein interactions, structure-function relationships, intramolecular gas diffusion, and metallocluster electronic structure.

Experiments identified multiple pathways for H_2 dispersion (Figure A) but only two major pathways for O_2 (Figure B) along the hydrogenase structure, suggesting that it is possible to mutate the protein to block O_2 access to the catalytic site without affecting the diffusion of H_2 product. Mutagenesis experiments revealed that substituting amino acid residues with larger residues results in mutated proteins that are more porous to oxygen.

Computational modeling with a different class of oxygen-accessible proteins, hemoglobins, allowed researchers to speculate that substituting smaller residues may be more favorable to decreasing oxygen accessibility by creating a less-flexible protein structure. This hypothesis is being tested now.



Study of high-capacity hydrogen storage in tetrahydrofuran-Li intercalated graphite

Significance of Accomplishments: Using computational science, NREL enhances the understanding of complex hydrogen research and accelerates its research pace. Computational modeling guides the experimental work, which feeds information back to prove or disprove the modeling-phase assumptions.

NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.
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