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Combining computation and experiment to accelerate the discovery of new hydrogen storage materials
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The potential of emerging technologies such as fuel cells (FCs) and photovoltaics for environmentally-benign power generation has sparked renewed interest in the development of novel materials for high density energy storage. For applications in the transportation sector, the demands placed upon energy storage media are especially stringent, as a potential replacement for fossil-fuel-powered internal combustion engines – namely, the proton exchange membrane FC – utilizes hydrogen as a fuel. Although hydrogen has about three times the energy density of gasoline by weight, its volumetric energy density (even at 700 bar) is roughly a factor of six smaller. Consequently, the safe and efficient storage of hydrogen has been identified as one of the key materials-based challenges to realizing a transition to FC vehicles. This talk will present an overview of recent efforts at Ford aimed at developing new materials for reversible, solid state hydrogen storage. A tight coupling between first-principles modeling and experiments has greatly accelerated our efforts, and several examples illustrating the benefits of this approach will be presented.