Sabrina Krupenko

Abstract

The need for alternative energy storage systems is exacerbated both by global energy demand and the pressure to switch to renewable energy. Investigation into new solid-state materials paves the way for energy systems capable of assisting in energy adaptability. Electrides, crystalline solids with bare electrons occupying lattice sites, are promising ion storage materials for batteries and hydrogen fuel cells. These solid-state electride technologies have high predicted energy capacities and efficiencies. Electrides could be used in hydrogen fuel cells as solid-state hydrogen storage, a safer alternative to current high-pressure, gaseous hydrogen fuel cells. Y_6S_4 is a promising electride for ion storage and conduction. In this work, we computationally and experimentally investigated Y_6S_4 as a hydrogen storage system. Computationally, we studied the structure and relative energy of different yttrium sulfide hydride (YSH) phases and the mobility of hydrogen through the structure. Multiple YSH phases are stable and the barrier for hydrogen diffusion is low (140.59 meV), which would make it a viable ion conductor. Experimentally, we have successfully synthesized Y_6S_4 and are developing a method for hydrogenation. The use of Y_6S_4 in a solid-state hydrogen fuel cell could create more compact, energy-dense storage materials that could potentially outperform commercial technologies and satisfy global energy demands.