INVESTIGATION OF HYDROGEN STORAGE AND DIFFUSION IN Y_6S_4

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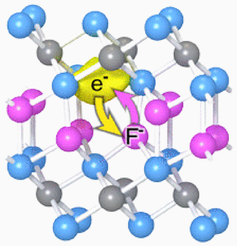
Background

Electrides

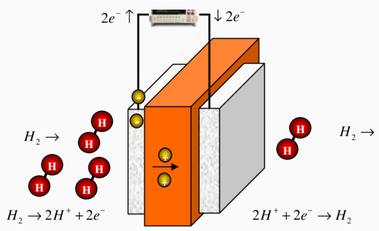
Electrides are crystalline solids that have electrons occupying lattice sites rather than within atoms. These are anionic electrons or bare electrons.



Electron-Anion Exchange

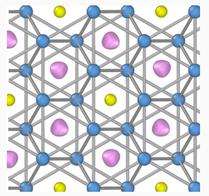
Typically, the gain or loss of electrons in a material must be accompanied by the reduction or oxidation of the atoms involved. In electrides, electrons and anions can be exchanged reversibly at room temperature. The net result of an EAX reaction is that atoms in the host lattice are neither oxidized nor reduced.

Hydrogen Fuel Cells

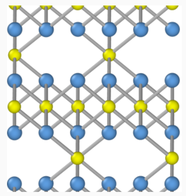


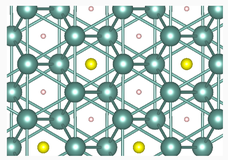
Hydrogen fuel cells (HFCs) generate electricity through a chemical reaction between Hydrogen and Oxygen, with water as the only by-product. Typically, HFCs require low temperatures and high pressure to store gaseous Hydrogen. Our work is motivated by the investigation into solid-state HFCs, which utilize a metal hydride to release and reabsorb hydrogen in its lattice structure. This project investigates the use of Yttrium Sulfide as hydrogen storage for a solid-state HFC metal hydride.

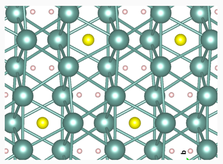
Y_6S_4-H

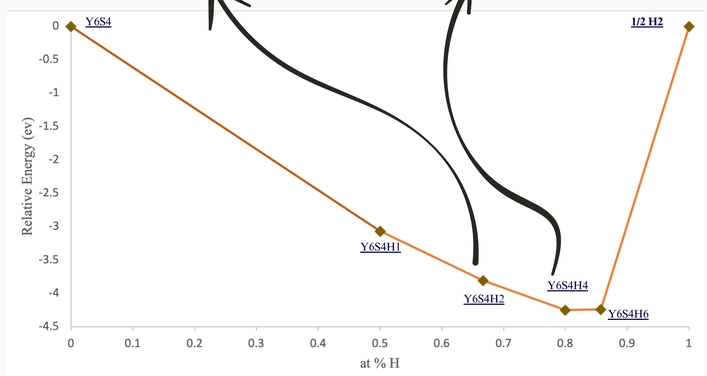


The lattice structure of Y_6S_4 indicates regions of electron density in octahedral sites. The structures of $Y_6S_4H_2$ and $Y_6S_4H_4$ indicate Hydrogen intercalates into the octahedral sites of the crystal lattice.

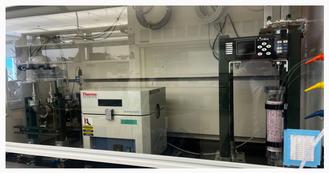




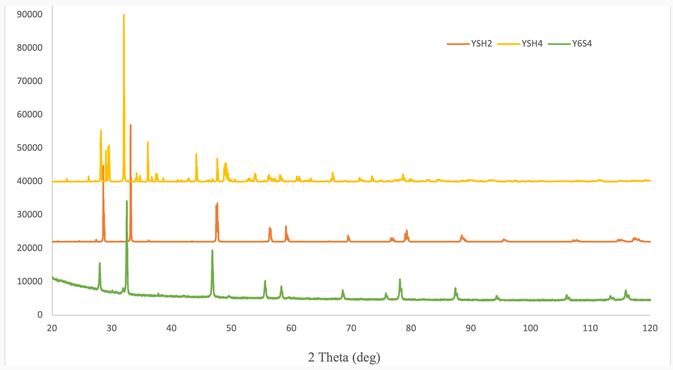




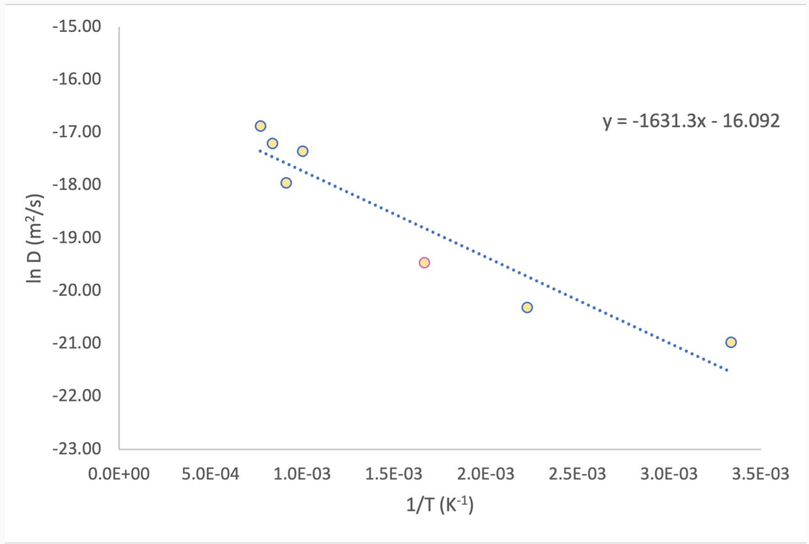
Synthesis and Characterization



Y_6S_4 was synthesized via arc melting and annealed at 1100 C for seven days. The method for hydrogenation will be a gas-phase reaction at elevated temperatures with H_2.



Molecular Dynamics



$$D = D_0 \exp\left(-\frac{E_a}{RT}\right)$$

Using the Arrhenius equation, we found that the activation energy for $Y_6S_4H_2$ is equal to 140.59 meV.

Future Work

Computational

Molecular dynamics calculations will be run to determine diffusion coefficients of different YSH structures.

Experimental

A method for hydrogenation will be developed and refined under different reaction conditions. Once synthesized, the ionic conductivity of YSH will be tested experimentally to verify its capability to be used as Hydrogen storage for a HFC.

References

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2. Schematic of solid state hydrogen pump or extractor. (n.d.). Retrieved April 21, 2023, from https://www.researchgate.net/figure/Schematic-of-solid-state-hydrogen-pump-or-extractor_fig5_41479928