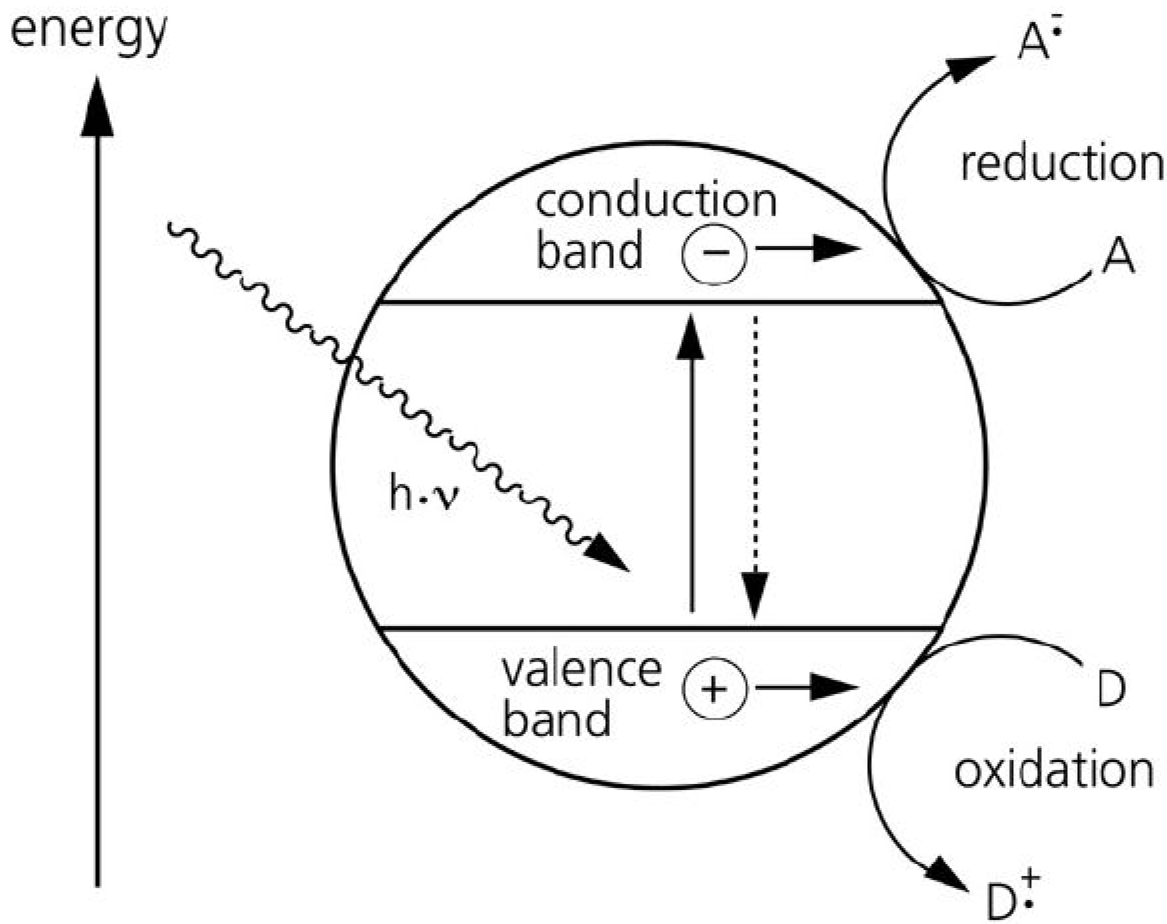
Senior Thesis Proposal

Introduction

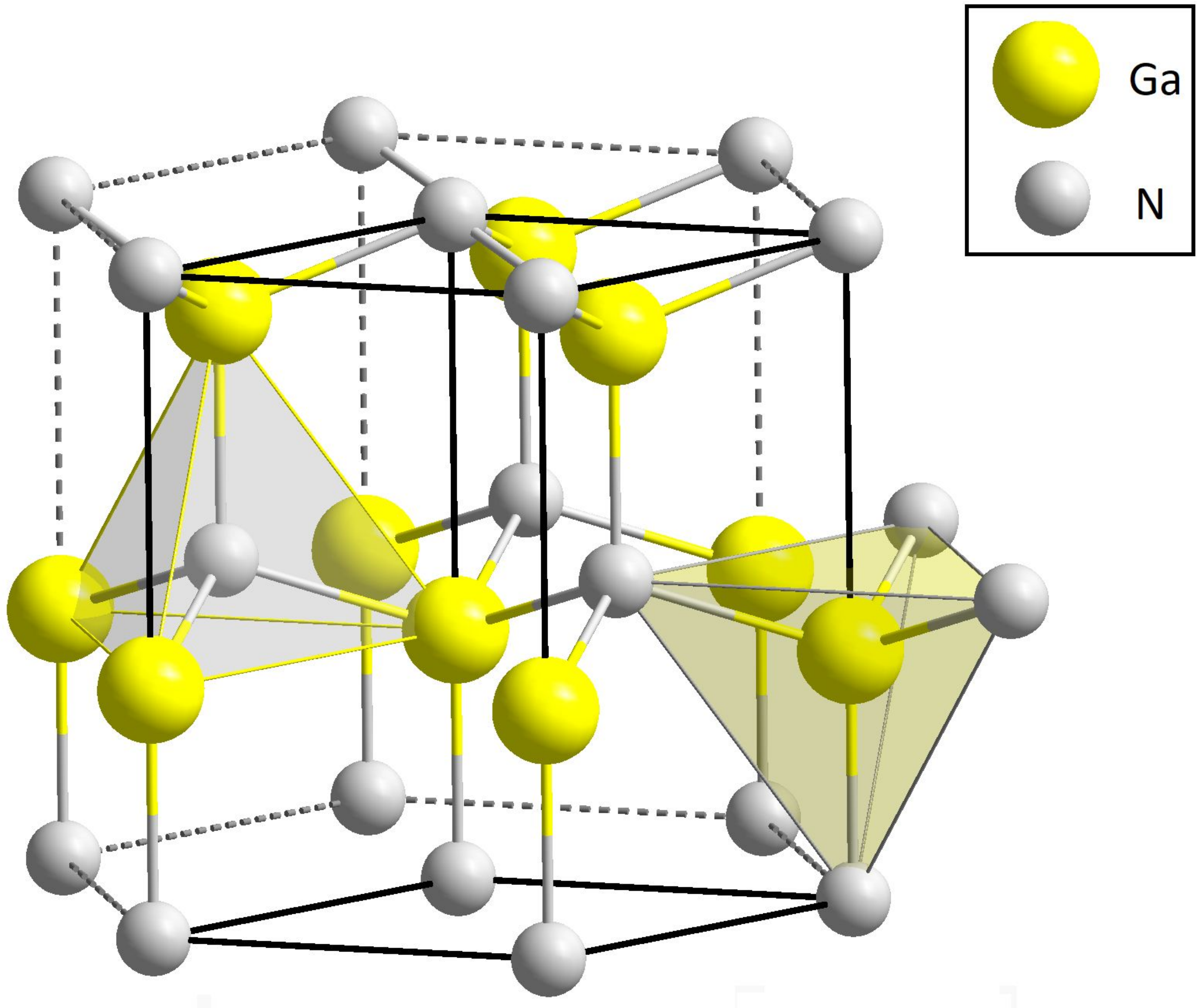
Ammonia is one of the most important chemicals in modern society, as it is essential in supporting the large scale agricultural practices that feed most of the human population on earth. Currently, the production of Ammonia is achieved with the Haber Bosch process, which captures and reduces atmospheric nitrogen gas to create ammonia. However, the Haber-Bosch process requires high temperatures (400-500 degrees celsius) and high pressures (150-300 atmospheres). It is extremely detrimental to the environment, and directly consumes around 2% of the world's energy production. Moreover, the production of the Hydrogen gas required for the Haber-Bosch process releases tremendous amounts of carbon dioxide into the atmosphere, contributing greatly to the growing trend of global warming.

An alternative approach to reduce nitrogen gas to ammonia involves electrochemical reduction, where the hydrogen for the reduction is obtained from water rather than hydrogen gas. With electrochemical reduction, the reaction can proceed at ambient pressures and temperatures, reducing production costs and environmental harm. Furthermore, the fine control permitted by electrochemical reduction would allow the thermodynamic equilibrium to be shifted toward the product side through adjustments to the electrode potential. However, electrochemical reduction is inefficient, especially in the hydrogen evolution reaction steps. A promising solution is to use electrocatalytic materials to expedite this process.

The idea is to enable a photo-driven reaction using a semiconductor electrode as a photocatalyst. With enough energy, incident photons will generate electron-hole pairs that can be utilized for reduction and oxidation reactions on the surface of the electrode.



Gallium Nitride
Gallium Nitride is a relatively new semiconducting material with many interesting properties. It’s band gap is roughly 3 times higher than that of silicon, and it also has a much higher resistance to temperature. This means that Gallium Nitride transistors have a much higher breakdown voltage than silicon transistors, and can be made smaller, and also pushed further, with a much less restrictive cooling constraint. Commercially, Gallium Nitride has already been used to create blue LEDs and the blue ray.



Gallium Nitride has a Wurzite structure.

Research Question: Can we use Gallium Nitride as a photo driven electrocatalyst for nitrogen fixation through an associative nitrogen reduction pathway?

Theory

Density Functional Theory
Hartree Fock Equations

Methods

To investigate the favorability of associative nitrogen reduction pathways, we use density function theory (DFT) calculations to obtain free energy diagrams. These DFT calculations were performed using implementations in the Vienna ab initio Simulation Package (VASP)