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Transparent Conducting Sulfides

Sondra Wouch
Washington University in St. Louis

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Mentor: Cynthia Lo

Researchers are constantly looking for new transparent conducting materials for applications in photovoltaics and flexible electronics (photochromic windows, flexible solar cells for satellites, and cell phone screens). This projects focuses on analyzing a large group of binary sulfide compounds as potential transparent conducting materials (TCMs). Through ab initio computations, the electronic properties of 186 binary sulfides will be examined.

The sulfides for this project were found through Materials Project with restrictions on the energy above hull (less than 0.01 eV) and band gap (greater than 0.5 eV). The sulfides were also selected to not contain any oxygen. A program was written to identify and list all the binary sulfide compounds with information in Materials Project that fit the previous requirements. This program gave a list of the materials' names and their Materials Project ID number. The ID number is what is used to call the information from the Materials Project website to be run through the calculations to obtain the electronic properties. All of the chosen sulfides were run through density functional theory (DFT) calculations performed by Vienna Ab Initio Simulation Package (VASP).

The first and foremost electronic properties that were collected from the DFT calculations are mobility and conductivity. This is because these two properties are the most comprehensive indicators that a material will make a reasonable transparent conducting material.

Mobility decreases as carrier concentration increases because more electrons result in a greater electronic field, which then results in less electron mobility. Similarly, conductivity increases as carrier concentration increases because a greater number of electrons increases the conductivity of the material. As such, these are the sought after trends for potential transparent conducting sulfides.