# The Good Kind Of Doping

## Could doping semiconductors with Iron improve conductivity?

### WHAT AND WHY

Semiconductors are a widely-used and highly-sought-after material – constant research underway to find more materials, improve efficiency, reduce costs

Compound semiconductors more efficient, can operate at wider temperature ranges [1] – Copper-based semiconductors more recent; $Cu_2S$ first efficient thin solar film

Other Copper-based semiconductors – $CuFeS_2$ well-researched and understood, Iron-doped systems less known about [2]

Copper Aluminium Iron Sulfide $CuAl_{(1-x)}Fe_{(x)}S_2$

- COMPOSITION
- STRUCTURE

→ PROPERTIES

### METHOD

**Step One: Which atoms?**

VMD software [3] used to visualise structure and find bond lengths between atoms

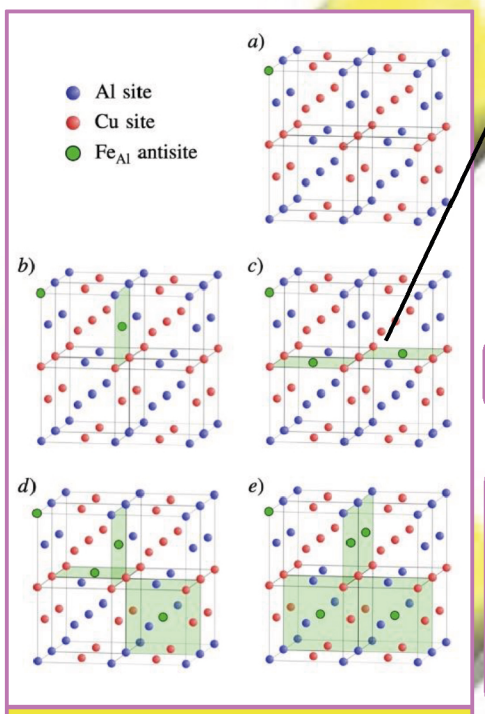


*Figure 1: Diagram displaying Fe defects within $CuAl_{(1-x)}Fe_{(x)}S_2$ for various x values*

Atoms in the system were chosen for uniform spacing

Uniform spacing

=

Uniform energy

**Step Two: Doping method**

Two methods:

- Replace Aluminium directly with Iron
- Replace Aluminium with Copper, then the closest Copper atom with Iron

**Step Three: Simulation & Analysis**

PBE Density Functional Theory (DFT) modelling method – this method of simulation provided lots of information about electronic structure of the material

*Figure 2: Equation to calculate formation energy*

$$\Delta H_D = (E_{Defect} - E_{Base}) + q(E_V - E_F) + \sum_j n_j(\mu_j + \Delta\mu_j)$$

Python used to calculate formation energies and plot "Density Of State" (DOS) graphs

### RESULTS

Filled sections → Energy states filled → No availability for extra electrons

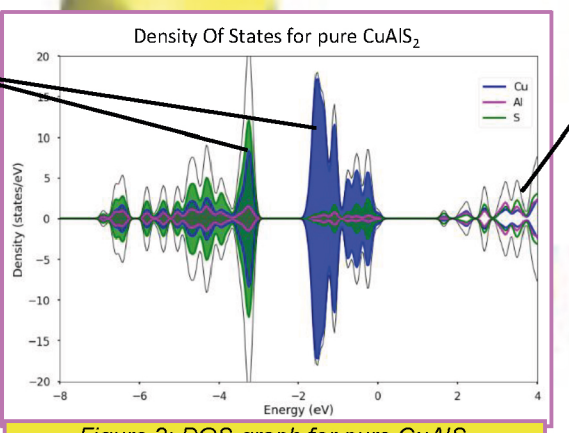


*Figure 3: DOS graph for pure $CuAlS_2$*

Empty sections → Energy states unfilled → Electrons may move into states

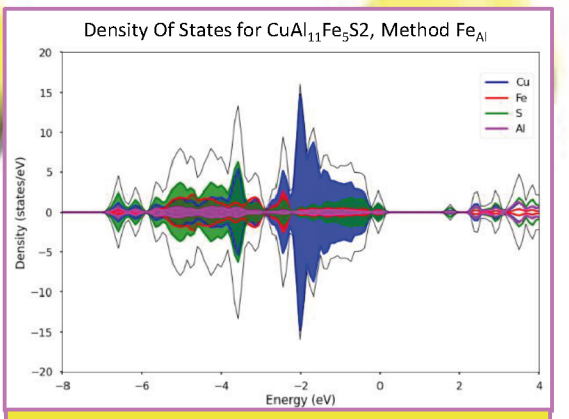


*Figure 4: DOS graph for $CuAlFeS_2$ with 5 defects, "direct doping" method used*

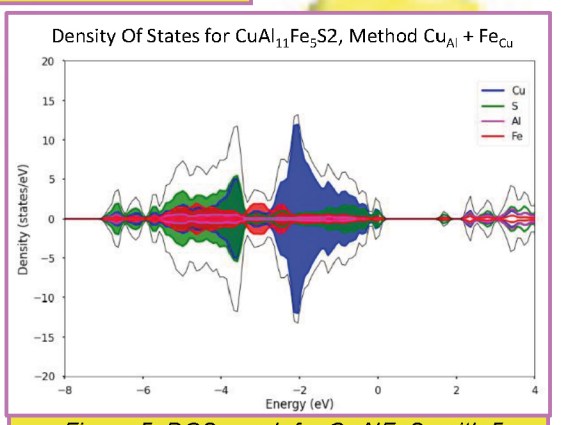


*Figure 5: DOS graph for $CuAlFeS_2$ with 5 defects, "indirect doping" method used*

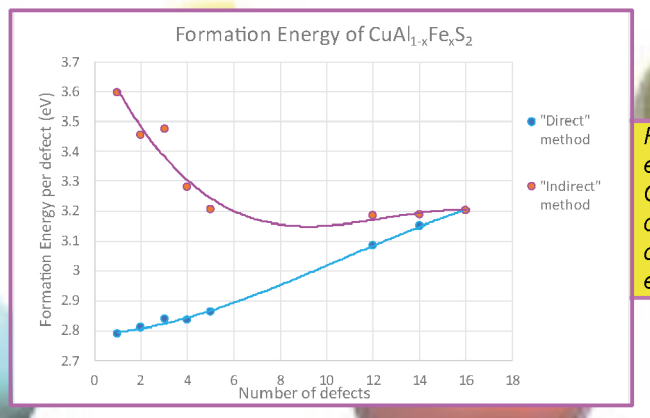


*Figure 6: Formations energies for various $CuAlFeS_2$ systems, compared against defect number for each doping method*

### CONCLUSIONS

Significant changes in DOS as no. Iron defects (x) increased – implies significant changes in conductivity for a doped system (in comparison to pure $CuAlS_2$ / $CuFeS_2$)

Similar DOS for each doping method – main difference is formation energies.

**"Direct" doping:** Lower initial formation energy - linear increase as x increases

**"Indirect" doping:** Higher initial formation energy, drops quickly – may be more beneficial in larger systems with higher x values

DFT (PBE) simulation method less accurate in determining band gaps – important property in semiconductors. Accurate band gaps would have been beneficial for determining efficiency changes

Future research:

- Synthesizing $CuAlFeS_2$ materials and testing them to compare against simulation
- Using different simulation methods to gain more insight into band gap changes


*ferences:* [1] S. F. Fang *et al.*, "Gallium arsenide and other compound semiconductors on silicon," *Journal of Applied Physics*, vol. 68, no. 7, pp. R31–R58, Oct. 1990, doi: 1063/1.346284. [2] S. Conejeros, P. Alemany, M. Llunell, I. de P. R. Moreira, SánchezV., and J. Llanos, "Electronic Structure and Magnetic Properties of $CuFeS_2$," *Inorganic Chemistry*, . 54, no. 10, pp. 4840–4849, May 2015, doi: 10.1021/acs.inorgchem.5b00399. [3] W. Humphrey, A. Dalke, and K. Schulten, "VMD: Visual molecular dynamics," *Journal of Molecular aphics*, vol. 14, no. 1, pp. 33–38, Feb. 1996, doi: 10.1016/0263-7855(96)00018-5.



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