Dopability of complex diamond-like semiconductors: new candidates for thermoelectric applications.

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Defects play a key role in thermoelectric semiconductors, which must be dopable to a significant degree for good performance. While recent developments in computational prediction have made good progress for thermoelectric materials discovery, prediction of dopability in complex materials remains a challenge. Of particular interest are the diamond-like semiconductors (DLS), a group that have recently garnered interest for the potential use as thermoelectric materials [1,2] but for which clear understanding of defect chemistry is still lacking.

In this work, we show our recent efforts to investigate the defect physics of a subset of materials within the DLS group formed by the ternary tellurides $\{Cu,Ag\}\{Ga,In\}Te_2$ using density functional theory (DFT). We show that there is a large diversity in the phase stability and in the range of achievable carrier concentrations under different growth environments. For example, CuXTe2 changes from a strongly p-type to an intrinsic material by changing the cation ion X from Ga to In (CuGaTe2 → CuInTe2).

Overall, the ternary tellurides show dopability windows ranging from highly p-type to intrinsic or slightly n-type. Control of carrier concentrations may then be achieved by growth under different thermodynamic environments, which is the focus of ongoing experimental work. We also highlight the importance of first-principles methods for accurate prediction of carrier concentrations, that can be used to guide further experimental works.

Finally, we present VTAnDeM (Visualization Toolkit for Analyzing Defects in Materials), a post-processing plotting toolkit for DFT calculations of defects in semiconductors. The script imports DFT data provided by users and produces phase stability diagram, defect diagrams, and carrier concentrations within an interactive user interface.

[1] Adv. Mater. **24**, 3622 (2012).
[2] AIP Advances. **5**, 107230 (2015).