First Principles Calculation of Optical Properties of Ternary Semiconductors Cu₃PSe₄ and Cu₃PS₄

DAVID FOSTER, GUENTER SCHNEIDER, Oregon State University — The ternary semiconducting compounds Cu₃PSe₄ and Cu₃PS₄ are of interest as potential optoelectronic materials. Of particular interest for solar photovoltaic devices is Cu₃PSe₄, as its band gap lies in the desired 1.0 to 1.6 eV range for an absorber. We have theoretically calculated the optical properties of these materials using density functional theory with GGA and hybrid exchange-correlation functionals, as well as with the GW₀ approximation from many-particle theory. We find that Cu₃PSe₄ has a direct band gap with relatively strong optical absorption above 2 eV, indicating that this compound is a candidate photovoltaic absorber. Cu₃PS₄ has a larger band gap of approximately 2.4 eV, placing it outside consideration as a solar absorber.

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Date submitted: 19 Nov 2010

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