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First Principles Calculation of Optical Properties of Ternary Semiconductors Cu_3PSe_4 and Cu_3PS_4 DAVID FOSTER, GUENTER SCHNEIDER, Oregon State University — The ternary semiconducting compounds Cu_3PSe_4 and Cu_3PS_4 are of interest as potential optoelectronic materials. Of particular interest for solar photovoltaic devices is Cu_3PSe_4, 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 GW_0 approximation from many-particle theory. We find that Cu_3PSe_4 has a direct band gap with relatively strong optical absorption above 2 eV, indicating that this compound is a candidate photovoltaic absorber. Cu_3PS_4 has a larger band gap of approximately 2.4 eV, placing it outside consideration as a solar absorber.

David Foster
Oregon State University

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