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Prediction of novel, Earth abundant Cu2O based alloys for PV applications[1] VLADAN STEVANOVIC, Colorado Sch of Mines, STEPHAN LANY, National Renewable Energy Laboratory — Tuning the opto-electronic properties of semiconductors through alloying is essential for semiconductor industry. Currently, mostly isovalent and isostructural alloys are used (e.g. Si/Ge, GaN/InN or CdTe/ZnTe), but a vast and unexplored space of novel functional materials is conceivable when considering more complex alloys by mixing aliovalent and heterostructural constituents. The real challenge lies in the quantitative property prediction for such complex alloys to guide their experimental exploration. In our work we demonstrate how an Earth abundant p-type oxide Cu2O, can be engineered through alloying into a technologically useful absorber material. We use non-local external potentials (NLEP) fitted to GW calculations for correcting the DFT electronic structure and compute absorption coefficient of different alloy compositions and configurations.

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