Thermodynamics of semiconductor doping and stoichiometry from first-principles methods\textsuperscript{1} STEPHAN LANY, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, CO 80401 — The theoretical investigation of semiconductor doping involves assessment of opposing physical effects: While extrinsic doping can shift the Fermi level in the desired direction, such shifts disturb the balance between intrinsic defects (vacancies, interstitials, etc.) leading to the creation of “killer-defects” and, in some materials, to considerable deviation from ideal stoichiometry. We have developed a self-consistent procedure which uses first-principles calculated formation enthalpies of impurities and intrinsic defects, to predict the correlation between doping, stoichiometry, and equilibrium carrier density. With this method, we explore the deviation from ideal stoichiometry and the electrical properties of the photovoltaic materials CuInSe\textsubscript{2} and CuGaSe\textsubscript{2}, sampling the entire space of thermodynamical variables. We find a systematic correlation between stoichiometry and conductivity type, which in case of CuInSe\textsubscript{2} spans the whole range from p- to n-type. Application to the case of N-doping of ZnO, identifies the narrow window for growth conditions that lead to p-type doping by N\textsubscript{O} acceptors.

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