Property optimization in isovalent and aliovalent semiconductor alloys based on MnO[1] HAOWEI PENG, STEPHAN LANY, National Renewable Energy Laboratory — Materials for solar energy conversion need to fulfill specific targets in regard of the band-structure, optical properties, carrier transport, and doping. In order to design or discover novel materials that satisfy multiple requirements, we employ design principles to select a range of material compositions where those properties are likely to occur, and then evaluate them computationally. Here we are addressing the design of semiconductor alloys based on the d^5 oxide MnO, which was recently identified as an interesting base material for semiconducting transition metal oxides [PRB 85, 201202(R)]. To calculate the properties for different alloy compositions with the many-body GW method, we modeled the alloy systems by searching for special quasi-random structures (SQS). In isovalent alloys, the SQS was chosen such that the correlation functions were as close as possible to the ideal random alloy. For aliovalent alloys where strong short-range-ordering is expected, the target correlation functions for the SQS search were determined by a Monte-Carlo simulation based on a cluster expansion of the total energy for the alloy. The optical properties determined from GW calculations for such SQS alloy structures are compared with available experimental data.

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