Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Thermochemical, structural and electronic properties of amorphous oxides, nitrides and sulfides PAWEL ZAWADZKI, STEPHAN LANY, National Renewable Energy Laboratory — Amorphous thin films materials become increasingly important components of many functional devices such as thin film displays, photovoltaic cells or thin film transistors. Due to lack of grain boundaries, they have superior uniformity and smoothest, flexibility and corrosion resistance. Amorphous thin films are typically prepared using physical vapor deposition (PVD) techniques at temperatures well below the melting point of deposited material (<0.2Tm). Computational models of amorphous structures, however, are almost elusively constructed from a high temperature equilibrated crystal melt using simulated annealing (SA) protocol. To account for low temperature growth conditions of amorphous thin films we recently developed a new simulation technique [1]. The method, kinetically limited minimization (KLM), starts from a randomly initialized structure and minimizes the total energy in a number of local structural perturbation-relaxation events. We apply KLM to model amorphous structures of 20 binary oxides, nitrides and sulfides and compare their thermochemical, structural and electronic properties.

[1] Zawadzki P., Perkins J., Lany S.; Modeling amorphous thin films: Kinetically limited minimization. Physical Review B **90** 094203 (2014)

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Date submitted: 12 Nov 2014 Electronic form version 1.4