Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Structure prediction for metastable materials: Sn_2N_2[1] STEPHAN LANY, National Renewable Energy Laboratory, Golden, CO 80401 — Recent advances in theoretical structure prediction methods and high-throughput computational techniques are revolutionizing experimental discovery of the thermodynamically stable inorganic materials. Metastable materials represent a new frontier for these studies, since even simple binary non-ground state compounds of common elements may be awaiting discovery. An interesting example of a metastable material is Sn_2N_2, a mixed valence Sn(II)/Sn(IV) tin nitride, which, due to its metastability relative to metallic Sn, N_2, and Sn_3N_4, remained elusive until recently [1]. This metastability presents a challenge for computational structure prediction, as common ground state search strategies are guided by energy minimization, which will eventually lead to a phase-separated configuration ($Sn+N_2$) instead of the desired Sn_2N_2 compound. Initial structure sampling has identified a number of candidate structures [1], but did not lead to an unequivocal assignment. We present the results of a new hybrid structure sampling approach predicting a bilayer structure with the possibility of polytypism. [1] C.M. Caskey *et al.*, J. Chem. Phys. 144, 144201 (2016).

[1]Supported by DOE-SC-BES (EFRC)

Stephan Lany
National Renewable Energy Laboratory, Golden, CO 80401

Date submitted: 20 Nov 2016 Electronic form version 1.4