Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Hybrid DFT calculations of the band structure of alpha-Sn ERIN DUPAY[1], LUCAS DOMULEVICZ[2], HENRY CASTEJON[3], AMJAD NAZZAL[4], Wilkes Univ — The electronic properties of bulk alpha-tin were revisited using first principles. The band structure, in addition to other properties, such as the absorption spectrum and density of states, were calculated using Density Functional Theory and the HSE06 hybrid functional. The direct and indirect band gaps obtained from these calculations are in better agreement with experimental results than previously reported calculations.

[1]Graduate Student
[2]Undergraduate Student
[3]Faculty
[4]faculty

Amjad Nazzal
Wilkes Univ

Date submitted: 06 Nov 2015 Electronic form version 1.4