Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

The benchmarking of density functional theory functionals with quantum Monte Carlo for an accurate description of thermoelectric materials AMANDA DUMI, JEFFRY D. MADURA, Duquesne University — A quickly progressing industrial and technological environment has necessitated the ability to create materials with tailored properties. Exploring new materials computationally has the potential to avoid the high cost of experimental synthesis. Density functional theory (DFT), a mean-field approach, is a prominent method for calculating accurate properties and energetics of solids. However, the choice of functional introduces uncontrolled approximations and often neglects dispersion effects. To describe materials with an accuracy necessary for consistent and reliable prediction, all relevant interactions must be captured. Quantum Monte Carlo (QMC), a statistical approach to solving the Schödinger equation exactly, can be utilized to address these shortcomings of DFT. In our work, QMC is utilized to benchmark DFT functionals, to obtain the most accurate results of transport properties in periodic solids viable for thermoelectric application. Here, we present results related to the study of tin selenide with QMC.

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Date submitted: 07 Feb 2017 Electronic form version 1.4