Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Ab Initio DFT study of electronic and thermoelectric properties of crystalline Ge2Sb2Te5[1] WILFREDO IBARRA HERNANDEZ, JEAN-YVES RATY, University of Liege — Pseudo-binary phase change materials such as (GeTe)n/(Sb2Te3)m have been recently considered for thermoelectric applications. Among these, Ge2Sb2Te5 (GST225, n=2 and m=1) is very popular as it is the leading candidate for non-volatile memory devices such as phase change random access memory. It is well know that the stable crystal structure of GST225 is hexagonal, with atomic layers stacked in the c direction. The stacking sequence is however still under some debate, and structures varying from conventional semiconductor to Dirac semimetal have been claimed to differ only by the nature of the stacking sequence. Here we present electronic, dynamic and thermoelectric calculations on three different stacking sequences of crystalline GST225. We use ab-initio DFT calculations together with Boltzmann transport equations to access thermoelectric properties within the constant relaxation time approximation. Our results show that all three proposed stacking sequences are (meta-)stable. From the density of states we determine that two structures are metallic while the most stable structure has a 0.35 eV band gap. Above 100K, the computed Seebeck coefficient seems to indicate that the experimentally observed structure is the Dirac semimetal one, the doping level being of the order of 1×1020 cm^{-3}.

[1]The authors acknowledge an A.R.C. grant (TheMoTherm 10/15-03) and the computer time provided by CECI, SEGI-ULg and PRACE projects NanoTherm (2IP FP7 RI-283493) and ThermoSpin on ARCHER (3IP FP7 RI-312763).

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Date submitted: 13 Nov 2014 Electronic form version 1.4