Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

How hybrid exchange affects thermoelectric transport properties of Cu2Se, III-V semiconductors, and half Heuslers: Accurate grid sampling enabled with a corrected k.p scheme.[1] KRISTIAN BERLAND, Univ of Oslo, OLE MARTIN LVVIK, Univ of Oslo, Sintef, CLAS PERSSON, Univ of Oslo — Accurate first-principle predictions of electronic transport (i.e. conductivity, Seebeck, etc.) is challenging to obtain. It demands both a good account of scattering and band structure. For Boltzmann transport calculations, the Brillouin zone needs to be sampled very densely, limiting the applicability of brute-force calculations with sophisticated methods such GW and hybrid functional calculations in density functional theory (DFT). Here we study the importance of the band structure by comparing results of hybrid and standard functionals. To make this comparison possible, we make use of a recently developed corrected k.p-based interpolation scheme that enables rapid convergence of the grid sampling [arxiv.org/abs/1607.01429]. The method is also applicable to properties such as density of states and dielectric functions. Beyond improving the band-gap issue, we show how using a hybrid functional based band structure can significantly impact the thermoelectric properties of direct band gap materials and materials with conduction and valence states with strong d-electron character. Further demonstrating the utility of the method, we present results a computational screening of the thermoelectric properties of a range of half Heusler compounds.

[1]THELMA project (Project no. 228854) supported by the Research Council of Norway.

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Date submitted: 11 Nov 2016 Electronic form version 1.4