PERFORMANCE OF GGA AND HYBRID FUNCTIONALS IN CALCULATION OF THERMAL CONDUCTIVITY OF Cu_2O

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One fundamental property of all materials is the conduction of heat energy. Depending on the application at hand, it is often necessary to either maximize it, or at least ensure sufficient conduction (heat extraction from electronic applications), or bring it down as much as possible (thermoelectrics).[1] Although the theory behind heat conductivity (κ) is well established, accurate tailoring of κ is still a bit of a far reach. With modern computational capacity it is already feasible to calculate and predict *ab initio* the thermal conductivity of simple Si and Ge to complex layered hybrid materials, which can guide materials design already in the early stages of research.[2, 3]

We present, to our knowledge, first lattice thermal conductivities calculated using hybrid density functional theory. We computed κ of Cu_2O with the GGA functional PBE and the hybrid funcional PBE0 using CRYSTAL14 and PHONO3PY[4], and found striking differences in performance. Earlier calculations have shown that PBE can produce satisfactory results when compared to experiment [3], but in the case of Cu_2O it results in an error of more than -40 %. PBE0, on the other hand, has an error of only around 7 % in the relevant temperature range ($\geq$ 300 K).

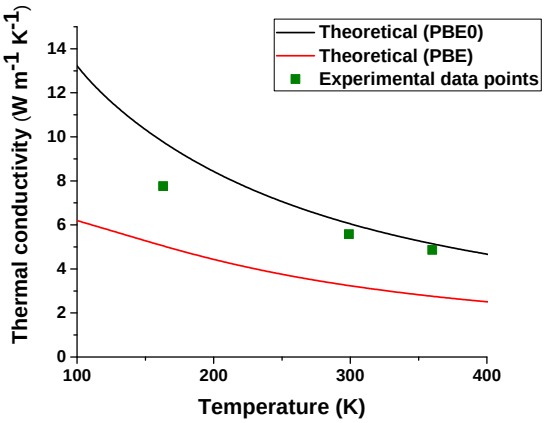

Figure 1: Thermal conductivity of Cu_2O between 100 and 400 K.

[1] E.S. Toberer, L.L. Baranowski and C. Dames, Annu. Rev. Mater. Res. 42 (2012), 179.
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[3] A.J. Karttunen, T. Tynell and M. Karppinen, Nano Energy 22 (2016), 338.
[4] A. Togo, L. Chaput and I. Tanaka, Phys. Rev. B. 91 (2015) 094306.