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High-throughput evaluation of descriptors for thermoelectric materials

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Achieving optimal carrier and minimal thermal conductivity is necessary for a given material to be suitable for thermoelectric energy conversion. Both properties are computationally too demanding for brute force approaches which demands that simplified descriptors are developed. Based on the recent computational discovery of favorable thermoelectric performance in the commercially viable an environmentally friendly Ag:SnS [1], we discuss how doping limits can be computationally screened. We will discuss the effects of two ubiquitous effects that can result in decreasing the hole concentration and show how the surprising results of Li doping can be rationalized based on data made available through on-line repositories. Furthermore, we show how the lattice thermal conductivity can be rapidly and reliably screened based on the quasi harmonic approximation [2]. We contrast this to the information covered by the available phase space for three-phonon scattering processes.

[1] Bera et al Phys. Chem. Chem. Phys.p19894, 16, 2014
[2] Bjerg et al Phys. Rev. B., p024304,89,2014