MAR15-2014-001664

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

**Modeling and Ab initio Calculations of Thermal Transport in Si-Based Clathrates and Solar Perovskites**[1]

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We present calculations of the thermal transport coefficients of Si-based clathrates [1,2] and solar perovskites [3], as obtained from ab initio calculations and models, where all input parameters derived from first principles. We elucidated the physical mechanisms responsible for the measured low thermal conductivity in Si-based clatherates [1] and predicted their electronic properties and mobilities, which were later confirmed experimentally [2]. We also predicted that by appropriately tuning the carrier concentration, the thermoelectric figure of merit of Sn and Pb based perovskites may reach values ranging between 1 and 2, which could possibly be further increased by optimizing the lattice thermal conductivity through engineering perovskite superlattices.

[1] Y. He and G. Galli, ***Nano. Lett.*** 14, 2920 (2014).
[2] Y. He, F. Sui, S. M. Kauzlarich and G. Galli, ***Energy Environ. Sci.***7, 2386 (2014).
[3] Y. He and G. Galli, ***Chem. Mat.*** 26, 5394 (2014).

[1]Work done in collaboration with Prof. G. Galli, and supported by DOE/BES grant No. DE-FG0206ER46262