Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

High throughput solution of Boltzmann transport equation: phonons, thermal conductivity and beyond JOSE PLATA, PINKU NATH, DEMET USANMAZ, Duke University, CORMAC TOHER, Duke Univ, MARCO FORNARI, Central Michigan University, MARCO BUONGIORNO NARDELLI, University of North Texas, STEFANO CURTAROLO, Duke University — Quantatively accurate predictions of the lattice thermal conductivity have important implications for key technologies ranging from thermoelectrics to thermal barrier coatings. Of the many approaches with varying computational costs and accuracy, which have been developed in the last years, the solution of the Boltzmann transport equation (BTE) is the only approach that guarantees accurate predictions of this property. We have implemented this methodology in the AFLOW [1] high throughput materials science framework, which enables us to compute these anharmonic force constants and solve BTE to obtain the lattice thermal conductivity and related properties automatically in a single step. This technique can be combined with less expensive methodologies previously implemented in AFLOW [2] to create an efficient and fast framework to accelerate the discovery of materials with interesting thermal properties. [1] S. Curtarolo et al., Comp. Mat. Sci. 58, 218 (2012). [2] C. Toher, et. al, Phys. Rev. B 90, 174107, 2014

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Date submitted: 03 Nov 2015 Electronic form version 1.4