Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Assessing the thermoelectric properties of sintered compounds via high-throughput ab initio calculations SHIDONG WANG, Department of Mechanical Engineering and Materials Science, Duke University, ZHAO WANG, LITEN, CEA-Grenoble, 17 rue des Martyrs, 38054 Grenoble Cedex 9, France, WAHYU SETYAWAN, Department of Mechanical Engineering and Materials Science, Duke University, NATALIO MINGO, LITEN, CEA-Grenoble, 17 rue des Martyrs, 38054 Grenoble Cedex 9, France, STEFANO CURTAROLO, Department of Mechanical Engineering and Materials Science and Department of Physics, Duke University — In order to identify promising thermoelectric materials, we study several thousand compounds from the ICSD database. In particular, we consider nanograined sintered power thermoelectric compounds with the high-throughput *ab initio* AFLOW framework (http://aflowlib.org and http://materials.duke.edu/aflow.html). By regression analysis, we find that the power factor is positively correlated to electronic band gap, carrier effective mass, and the number of atoms per unit cell. This work illustrates the important role that experimental and theoretical databases can play in the development of novel materials.

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Date submitted: 26 Nov 2011 Electronic form version 1.4