Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Thermoelectric properties of correlated materials JAN TOMCZAK, KRISTJAN HAULE, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA, TAKASHI MIYAKE, Nanosystem Research Institute, AIST, Tsukuba 305-8568, Japan, ANTOINE GEORGES, Centre de Physique Theorique, Ecole Polytechnique, CNRS, 91128 Palaiseau Cedex, France, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — The discovery of large Seebeck coefficients in transition metal compounds such as FeSi, FeSb2, or the iron pnictides, has stirred renewed interest in the potential merits of electronic correlation effects for thermoelectric properties. The notorious sensitivity in this class of materials to small changes in composition (doping, chemical pressure) and external stimuli (temperature, pressure), makes a reliable and, possibly, predictive description cumbersome, while at the same time providing an arena of possibilities in the search for high performance thermoelectrics. Based on state-of-the-art electronic structure methods (density functional theory with the dynamical mean field theory) we here compute the thermoelectric response for several of the above mentioned exemplary materials from first principles. With the ultimate goal to understand the origin of a large thermoelectricity in these systems, we discuss various many-body renormalizations, and identify correlation controlled ingredients that are pivotal for thermopower enhancements.

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Date submitted: 23 Nov 2010 Electronic form version 1.4