

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Unusual Transport and Strongly Anisotropic Thermopower in PtCoO₂ and PdCoO₂ KHUONG ONG, Institute of High Performance Computing, DAVID SINGH, Oak Ridge National Laboratory, PING WU, Institute of High Performance Computing — Thermoelectrics provide a technology for producing electrical energy from solar and other heat sources. Thermoelectric performance requires materials with high thermopower, normally found in doped semiconductors, where the thermopower is generally nearly isotropic. We discovered using first principles calculations and Boltzmann transport theory that two oxides, PtCoO₂ and PdCoO₂, which are not semiconductors, but rather good metals, have exceptionally large thermopowers in one direction, and moreover that the thermopower in these materials is highly anisotropic. This places these compounds in a highly unusual transport regime. Besides providing a new direction for thermoelectric materials research, they may be very useful in probing the fundamental limits of conventional transport theory for metals.

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Date submitted: 10 Nov 2010

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