

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

**Quantum-Enhanced Thermoelectric Effects
in Polycyclic Molecular Junctions**¹ JOSHUA BARR, CHARLES
STAFFORD, University of Arizona — We calculate the thermoelectric
response of a polycyclic molecular junction including electron-electron
interactions. To do this, the molecular Green's function is determined
via a Lanczos-based technique and π -electron effective field theory is
used to model the degrees of freedom most relevant to transport. In these
junctions we find that the presence of multiple rings leads to higher order
quantum interference features giving rise to dramatic enhancements
of molecular thermoelectric effects, consistent with previous predictions
based on Hückel theory, which neglected electron correlations.

¹This material is based upon work supported by the Department of
Energy under Award Number DE-SC0006699.

Joshua Barr
University of Arizona

Date submitted: 11 Nov 2011

Electronic form version 1.4