

Abstract Submitted
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Thermoelectricity and transmission eigenchannels in buckyball junctions¹ MICHAEL STEFFERSON, JARRED HUDSON, JOSHUA BARR, Department of Physics, University of Arizona, JUSTIN BERGFELD, Department of Chemistry, Northwestern University, CHARLES STAFFORD, Department of Physics, University of Arizona — Transmission through nanoscale junctions consisting of a single Buckminsterfullerene molecule between two Pt or Au electrodes is investigated in the Coulomb blockade regime using the nonequilibrium Green's function approach. The Green's function of the buckyball is calculated in the isolated-resonance approximation, including the degenerate HOMO and LUMO orbitals. Electron-electron interactions were included in a constant-interaction model derived from π -electron effective field theory. For junctions with Pt electrodes, we find two transmission channels (despite the 5-fold degenerate HOMO and 3-fold degenerate LUMO resonances) and a positive thermopower. For Au electrodes, the thermopower is strongly affected by quantum interference, and we find just one transmission channel.

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