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The number of transmission channels through a single-molecule junction STAFFORD CHARLES, JUSTIN BERGFELD, JOSHUA BARR, University of Arizona — We calculate transmission eigenvalue distributions for Pt-benzene-Pt and Pt-butadiene-Pt junctions using realistic state-of-the-art many-body techniques. An effective field theory of interacting pi-electrons is used to include screening and van der Waals interactions with the metal electrodes. We find that the number of dominant transmission channels in a molecular junction is equal to the degeneracy of the molecular orbital closest to the metal Fermi level. Thus for Pt-benzene-Pt junctions we predict two dominant transmission channels, and for Pt-butadiene-Pt junctions only one. Pt-buckyball-Pt junctions are predicted to exhibit up to five dominant transmission channels.

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