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Finding Destructive Interference Features in Molecular Transport Junctions MATTHEW REUTER, Institute for Advanced Computational Science and Department of Applied Mathematics & Statistics, Stony Brook University, THORSTEN HANSEN, Department of Chemistry, University of Copenhagen — Associating molecular structure with quantum interference features in electrode-molecule-electrode transport junctions has been difficult because existing guidelines for understanding interferences only apply to conjugated hydrocarbons. Herein we use linear algebra and the Landauer-Büttiker theory for electron transport to derive a general rule for predicting the existence and locations of interference features. Our analysis illustrates that interferences can be directly determined from the molecular Hamiltonian and the molecule-electrode couplings, and we demonstrate its utility with several examples.

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