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Quantum-Interference-Controlled Molecular Electronics SAN-HUANG KE, WEITAO YANG, H. U. BARANGER, Duke University — Quantum interference in coherent transport through single molecular rings may provide a mechanism to control the current in molecular electronics. We investigate its applicability, using a single-particle Green function method combined with *ab initio* electronic structure calculations. We find that the quantum interference effect (QIE) is strongly dependent on the interaction between molecular π-states and contact σ-states. It is masked by σ tunneling in small molecular rings with Au leads, such as benzene, due to strong $\pi - \sigma$ hybridization, while it is preserved in large rings, such as [18]annulene, which then could be used to realize quantum interference effect transistors. [Nano Letters 8, 3257 (2008)]

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