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Title: Chemically Gated Quantum-Interference-Based Molecular Transistor

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Source title: JOURNAL OF PHYSICAL CHEMISTRY LETTERS

Volume: 2 Issue: 14

pages: 1753-1756

Publication year: JUL 21 2011

Abstract: This Letter proposes a realistic design of a single-molecule quantum-Gate interference-based transistor. The transistor consists of a cross-conjugated donor-bridge-acceptor molecule and is chemically gated by a functional group that can be charged. Numerical simulations indicate that the device properties can be tuned to desired specifications by the choice of its constituting functional groups. The transistor does not require external contacts to control its operation. However, it can be chemically functionalized for easy integration into molecular electronic circuits, especially because its operation does not involve any conformational changes in the molecule. The upper operational frequency limit of the proposed device is found to be in the terahertz range.