

Abstract Submitted
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Trends in Conductance through Single Molecule Junctions Formed with Double-Layered Molecules¹ HECTOR VAZQUEZ, MASHA KAMENETSKA, JONATHAN WIDAWSKY, RACHID SKOUTA, SEVERIN SCHNEEBELI, RONALD BRESLOW, MARK S. HYBERTSEN, LATHA VENKATARAMAN — We compare experimentally measured single-molecule conductances with Density-Functional Theory (DFT) based calculations for a series of “double-decker” molecules in which two parallel backbones are held between a common contact group on each end, consisting of S(CH₂)₂ units. In the simplest example, the two backbones are both phenyl groups, but an extensive series has been studied in which one or both parallel backbones are varied to include either short alkane segments, phenyl groups with substituents or fluorenes. Single molecule transport measurements using the STM-break-junction technique reveal that these molecules have multiple conducting states, suggesting that the single molecule junction geometry plays an important role in the outcome of these experiments. Density Functional Theory based calculations are used to explore the role of the link geometry on the conductance and to understand the relationship between the double-decker structure and the conductance.

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