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Electron transport through molecular-carbon nanotube interfaces NICOLAS BRUQUE, RAJEEV PANDEY, KHAIRUL ALAM, ROGER LAKE, UC Riverside — Investigations have focused on electron transport through metal-molecule systems. Less effort has been directed towards semiconductor-molecule systems, and the least attention has been given to electron transport through carbon nanotube-molecule systems. A specific implementation of the latter system consists of two CNTs joined by a molecule, or a CNT-molecule-CNT system. Such a system can provide the electronic functionality of a resonant tunnel diode. The molecular contacts, i.e. the CNTs, are a π-bond surface and, as such, they are both chemically and geometrically different from metal contacts or sp^3 semiconductor contacts. A model system is studied to focus solely on the interface geometry of two simple π-bond systems, CNTs and polyacetylene $(CH)_n$. The system is CNT-$(CH)_n$-CNT. At the interface, in the relaxed structure, the $(CH)_n$ is oriented coplanarly with the tangential plane of the CNT. The transmission, calculated with our DFT (FIREBALL)-NEGF code is, on average, 3 or more orders of magnitude larger than the transmission of an unrelaxed structure in which the $(CH)_n$ is perpendicular to the CNT at the point of contact. This is also true when the $(CH)_n$ of the relaxed structure undergoes a 180^o twist. Interface geometry plays a crucial role in the electron transport.

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