COHERENT ELECTRON TRANSPORT THROUGH A MOLECULAR NANO-JUNCTION: A LIGHT-DRIVEN MOLECULAR SWITCH

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We apply a first-principles computational approach to study a light-sensitive molecular switch. The molecule that comprises the switch can convert between a trans and a cis configuration upon photo-excitation. We find that the conductance of the two isomers vary dramatically, which suggests that this system has potential application as a molecular device. A detailed analysis of the band structure of the metal leads and the local density of states of the system reveals the mechanism of the switch. In addition, we also report our recently progress on the spin-dependent transport properties of nano-wires.