Exchange interaction in organometallic molecule induced for temperature

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We have performed theoretical calculations to investigate the electronic transport of a single metal-molecule sandwiched between two metallic gold contacts; specifically, in $(Fe\text{-}bpfp2)^{+2}$ the stability is obtained by linking the iron ion at the pyridine molecules.The nonequilibrium Green function is used to investigate the eletronic transport.The differential conductance *dI/dV* are monitored and we have obtained the transmission function *T (E,V)* and density of states *DOS*. Experimental realizations reveal dependence in the temperature for low bias regime [1] and our theoretical findings are also agree for description an organometallic molecule for low temperature. We theoretically calculate the conductance with the temperature dependence for 30k, 20K, 9K, 7K and 1.4K. The peak conductance for zero voltage increases with decreasing temperature indicating a peak Kondo and increases voltage reveals clearly a NDR. Interestingly, low temperature 9K, 7K and 1.4K) is observed a higher conductance voltage for 0.04V and a suppression in ZBP.The peak for 0.04V demonstrate a competition between superconductance and Kondo resonances, with in 1.4K observed a decrease in peak conductance for zero voltage against rising peak conductance in 0.04V. The absence of superconductance in 20k 30k is attributed to the strong local magnetic moment that interacts with electrons conduction; by consequence the system displays a more pronounced peak kondo. On the other hand, the less peak kondo is attributed to the weak local magnetic moment causing a superconductance in 1.4k with increase voltages. Superconductance in a SMT was yet to be observed as it offers new insights into the couplings involved in single molecule junctions[2].

References:

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