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The first-principle study of single molecular switch based on Hydrogen Tautomerization sandwiched between atomic chain electrode J. PRASONGKIT, Condensed Matter Theory Group, Uppsala University, Sweden, A. GRIGORIEV, Uppsala University, Sweden, G. WENDIN, Chalmers University of Technology, Sweden, R. AHUJA, Uppsala University, Sweden — Using DFT based NEGF technique, we investigated electrical transport properties of the single-molecular switch, phthalocyanine (H2Pc), based on hydrogen tautomerization. The molecule is coupled to 1-D electrodes in the form of semi- infinite metallic chains of gold and carbon. Hydrogen tautomerization affects the electronic state of H2Pc by switching the alignment of the molecular orbital energies between HOMO and HOMO-1, and causes a substantial change in the tunnelling current. As a consequence switching can be achieved already in the low-bias regime for both electrode models. For gold chain electrode, molecule-metal interaction at the junction leads to modification of the electronic structure of H2Pc, and hence multi-peak NDR is obtained. It is revealed that the even-numbered Au atoms provide stronger NDR than odd- numbered Au atom. Owing to interesting switching characteristics of H2Pc based on hydrogen tautomerization, it could potentially function as a molecular switch in nano electronic circuits.

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