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Quantum current of a molecular photo-switch between two graphene sheets G.P. BRIVIO, C. MOTTA, Università di Milano-Bicocca, Italy, M.I. TRIONI, CNR, ISTM, Milano (Italy), K.L. SEBASTIAN, Indian Institute of Science, Bangalore (India) — Light responsive materials that reversibly change shape under alternate UV and visible irradiation have attracted much interest because they can be used as optical switches, since the isomers show different features in the dimension, HOMO-LUMO gap and transmission spectrum. In view to integrate the photo-switch in the carbon based electronics devices, the conductance of a system constituted by a photochromic molecule between two graphene electrodes is investigated. In this work the conductance of the junction formed by diarylperfluorocyclopentene between two semi-infinite graphene sheets was computed using the non-equilibrium Green's function method combined with density functional theory via the TranSiesta code. The results emphasize the role of the graphene and the molecular electronic states in the switching behaviour of this hybrid system.

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