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Electron Transfer Mechanism in Gold Surface Modified with Self-Assembly Monolayers from First Principles[1] FILIPE C. D. A. LIMA, IF-USP/Brazil, RODRIGO M. IOST, FRANK N. CRESPILHO, IQSC-USP/Brazil, MARÍLIA J. CALDAS, IF-USP/Brazil, ARRIGO CALZOLARI, CNR-NANO/Italia, HELENA M. PETRILLI, IF-USP/Brazil — We report the investigation of electron tunneling mechanism of peptide ferrocenyl-glycylcystamine self-assembled monolayers (SAMs) onto Au (111) electrode surfaces. Recent experimental investigations showed that electron transfer in peptides can occur across long distances by separating the donor from the acceptor. This mechanism can be further fostered by the presence of electron donor terminations of Fc terminal units on SAMs but the charge transfer mechanism is still not clear. We study the interaction of the peptide ferrocenyl-glycylcystamine on the Au (111) from first principles calculations to evaluate the electron transfer mechanism. For this purpose, we used the Kohn Sham (KS) scheme for the Density Functional Theory (DFT) as implemented in the Quantum-ESPRESSO suit of codes, using Vandebilt ultrasoft pseudopotentials and GGA-PBE exchange correlation functional to evaluate the ground-state atomic and electronic structure of the system. The analysis of KS orbital at the Fermi Energy showed high electronic density localized in Fc molecules and the observation of a minor contribution from the solvent and counter ion. Based on the results, we infer evidences of electron tunneling mechanism from the molecule to the Au(111).

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