Density Functional Theory Study of the Interaction of 2- Mercaptobenzimidazole and Gold, Palladium and Nickel atoms

Ourida Mahmoudi^{1, 2, 3}, Tarik Bordjiba^{2, 3 *} and Abed Mohamed Affoune³

¹Departement of Chemistry, Sciences Faculty, Badji-Mokhtar-Annaba University, Box 12 , 23000 Annaba, Algeria

²Laboratory of Electrical Engineering of Guelma, 8 mai 1945-Guelma University Box 401, 24000 Guelma, Algeria

³Process Engineering Department, Sciences and Engineering Faculty, 8 mai 1945-Guelma University, Box 401, 24000 Guelma, Algeria

*E-mail: bordjiba_tarik@yahoo.ca

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The purpose of this work is to study the adsorption of 2-Mercaptobenzimidazole on three different types of atoms: gold, palladium and nickel. The Density Functional Theory Study (DFT) calculations were performed on 2-Mercaptobenzimidazole (2MBI) and three complexes: 2-Mercaptobenzimidazole-gold atom (2MBI-Au), 2-Mercaptobenzimidazole-palladium atom (2MBI-Pd) and 2-Mercaptobenzimidazole-nickel atom (2MBI-Ni). The quantum chemical parameters of 2MBI and the complexes: 2MBI-Au, 2MBI-Pd and 2MBI-Ni, have been calculated. The considered quantum chemical parameters are: lengths bonds, angles bonds, optimization energy, binding energy, Mulliken atomic charges, energies of highest occupied molecular orbital (E_{HOMO}), the lowest unoccupied molecular orbital (E_{LUMO}), the energy difference (ΔE) between E_{LUMO} and E_{HOMO} , chemical hardness η and the dipole moment μ . The complexation of 2MBI with Au, Pd and Ni atoms modifies the quantum chemical parameters of the organic molecule. This study reveals that gold atom bonds with 2MBI molecule via sulfur atom, however, the palladium and nickel atoms bond with 2MBI molecule via nitrogen atom. The results of the present work give a new insight on self assembly of 2-Mercaptobenzimidazole molecules at metal surface and provide significant information for fundamental and applied electrochemistry.

Keywords: 2-mercaptobenzimidazole, self-assembly, Adsorption, Density Functional Theory (DFT), Energy gap, chemical hardness η , Dipole moment, Theoretical calculation, Gold, Palladium, Nickel.

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