

Abstract Submitted
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Peculiarity of Thiophene/Graphene interface for organic electronic applications SOURAYA GOUMRI-SAID, Al Faisal University — Interfacial study between thiophene molecule and graphene surface is investigated on the basis of density functional theory. The reported HOMO-LUMO energy gaps, adsorption energy as well as binding energy are showing the existence of intermolecular forces accumulated from the attractive van der Waals forces and Pauli repulsion forces. The interface's separation distance is varied from 1.00Å to 2.50Å. It is noted that, subsequently growing intermolecular forces are very sensitive even to a relatively small change in the interface's separation distance between the molecule and the surface. The electronic density of states, dense electrons population of the thiophene/graphene system is found to be at energy Fermi level with appearance of spin-polarization. A slight magnetic behaviour on thiophene molecule, accompanied by a decrease in the magnetization of graphene surface was observed in the presence of the molecule near to the surface.

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