Theoretical insight into stability of vanadium phthalocyanine adsorbed at graphene monolayer and gold surface

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Transition metals - phthalocyanines (TM-Pc's) grafted to suitable two-dimensional materials constitute perspective hybrid systems that potentially could be implemented as active parts of spintronic devices. In the present communication, we report our studies of vanadium phthalocyanine (V-Pc) adsorbed to graphene and gold (111) surface. Our studies are based on theoretical calculations in the framework of density functional theory within the supercell geometry, taking into account the spin polarization of the system and dispersive (Van der Waals) interactions between the layers. We pay particular attention to the stability of the adsorbed molecule and the change of the V-Pc magnetic moment as the result of grafting the molecule to the substrate. For both substrates, we consider various V-Pc adsorption sites at the surface and determine the energetically most favorable configuration. In the case of V-Pc on graphene, it is 'bridge' position with the central V atom of V-Pc placed between two C atoms, whereas the equilibrium position for V-Pc is such that V atom is at the so-called fcc position on the Au(111) lattice. The distances between V atom in the V-Pc molecule and the graphene and Au(111) surfaces are equal to 3.12 and 2.51 Å, respectively. Correspondingly, the binding of the V-Pc molecule to the graphene is weaker than to Au(111) surface, as quantified by the adsorption energies of V-Pc being equal to -4.11 and -5.42 eV, for graphene and Au(111) surface, respectively. It is interesting to point out that the van der Waals forces contribution to the adsorption energy is very large (being equal to -3.37 eV) for the case of V-Pc on Au(111) surface, and rather tiny in the case of V-Pc on graphene (being of the order of 0.03 eV).

The interesting issue is how the magnetic moment of the free standing V-Pc molecule changes after adsorption to the substrate. To illustrate these changes, we quote the calculated magnetic moments on the V atom. In the case of free standing V-Pc molecule, V-Pc on graphene, and V-Pc on Au(111) surface, the magnetic moment is equal to 2.88, 2.84, and 1.75 μ_B, respectively. Clearly, the stronger interaction of the V-Pc molecule with the Au(111) surface than with the graphene layer leads also to stronger changes of the magnetic moment. The relation between stability of the V-Pc/substrate hybrid structure and the induced changes of the magnetic moment is very important factor in design of magnetic memories based on such systems. Our calculations shed light on the physical mechanisms of interaction between adsorbate and adsorbent.

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