

Magnetic states of hybrid system built of iron phthalocyanine at Ti₂C layer

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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. The choice of substrate affects the magnetic properties of TMPc's. MXenes, fairly new family of 2D materials based on transition metal carbides and nitrides, were not studied yet as substrates in such hybrid systems. Here, we report the results of theoretical studies of the iron phthalocyanine (Fe-Pc) molecule adsorbed at the Ti₂C layer.

The most relevant issue in the present study is interaction between transition metals, from the molecule and the substrate. Special attention is paid to the issues of structural optimization and magnetic characteristics of this complex, where various magnetic configurations are considered. The ability of the surface to assume stable ferromagnetic and antiferromagnetic phases and the induced orientation change of the magnetic moment in the FePc lead to four different electronic configurations of the hybrid system, each exhibiting various properties. The significant ferromagnetic interaction between the iron atom and the upper titanium layer plays important role in the reorientation of the iron atom magnetic moment. We also analyze a model of the system in which the Fe-Pc molecule is in a quintet state (the ground state of an isolated molecule is a triplet). The calculations have been performed in the framework of density functional theory employing the plane waves and pseudo-potentials as implemented in the *Quantum Espresso* numerical package.

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