Single molecular magnets with single transition metal ion grafted to graphene monolayer: *ab initio* studies

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Single Molecular Magnets grafted to 2D structures can be considered as potential memory storage devices due to the possibility of preserving and changing the molecular spin. 2D materials, in turn, can act both as a substrate for molecules and as a means of changing the spin moment of molecules. In the present communication, we study molecular magnets with a single transition metal ion [Fe-Phthalocyanine (Fe-Pc) and a molecule with linear coordinated iron atom $Fe(C(SiMe_3)_3)_2$] as carriers of the spins and consider their interactions with the graphene surface. To study the described hybrid systems, we employ density functional theory (DFT) as implemented in *VASP* and *SIESTA* numerical packages GGA-PBE and VDW-DRSLL exchange-correlation functionals, and also the approximate scheme of density.

Our studies reveal the possibility of physisorption and also chemisorption of the two studied SMMs to the surface of graphene, however, the formation of the covalent bond between SMMs and graphene has dissociative character and happens only after the reaction of dehydrogenation of the SMMs molecules. The grafting of the SMMs to the graphene does not change its magnetic properties and magnetic moment remains mostly concentrated on the transition metal ion.

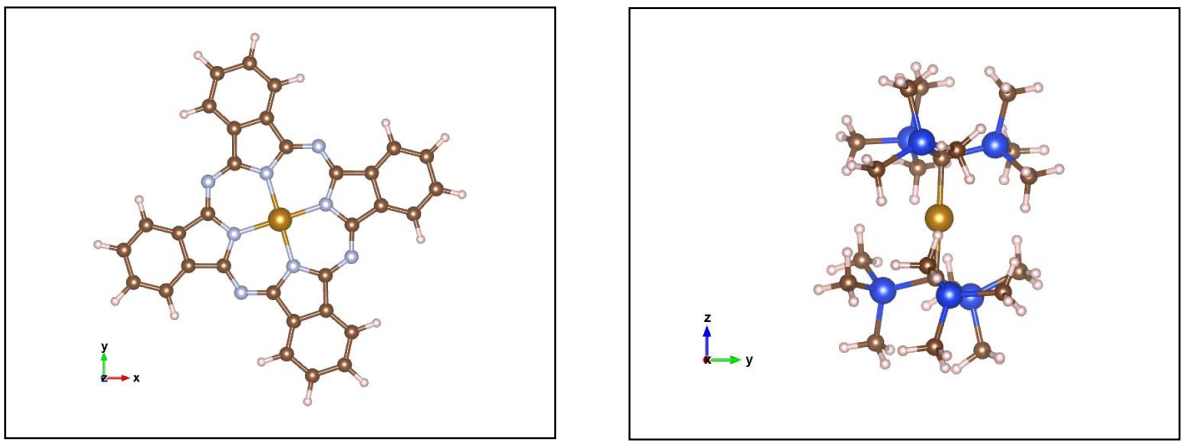

Figure: The Fe-Pc (left) and $Fe(C(SiMe_3)_3)_2$ (right) SMMs studies in the paper

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