# Comparative Theoretical Study of Adsorption of Vanadium Phthalocyanine on Graphene and Au(111) Surface

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The planar systems, such as graphene, silicene, hexagonal boron nitride, planar transition metal dichalcogenides exhibit intriguing properties, and at present are considered as the most promising candidates for future applications in the whole plethora of fields including nano-electronics, optoelectronics, and spintronics. The functionalization of these layered systems with molecular nanomagnets (e.g., with so-called single molecular magnets, SMM) can increase the number of functionalities exhibiting by these systems and lead to tunable array of magnetic nano-crystals on surface of a system, and then to the novel spin-based technologies.

In this communication, we study the electronic and magnetic properties of Vanadium phthalocyanine molecule (V-Pc) adsorbed on graphene and Au(111) surface. These studies are based on theoretical calculations within the density functional theory (DFT) employing the computer packages VASP [1] and SIESTA [2]. In particular we study adsorption energies of V-Pc molecules, the induced changes of the geometry of the system with grafted V-Pc molecule, and magnetic properties of the system, including the interaction between the SMM and the substrate. In both packages we use the generalized gradient approximation for exchange-correlation energy functional and van der Waals correction, however, the electron-ion interaction is accounted for employing projector augmented wave (PAW) and norm-conserving Troullier-Martins pseudopotentials in the VASP and SIESTA codes, respectively. Our studies reveal that the adsorption of the V-Pc molecule to both graphene and gold surface is possible and we determine the energetically most stable geometry of the grafted molecule. In particular, the most favorite adsorption site of V-Pc molecule to Au (111) surface is the fcc site as depicted in the Figure below. Our present work sheds light on physical mechanisms of the SMMs adsorption to half-metallic and metallic surfaces and opens up new prospects for design of novel spintronic devices.

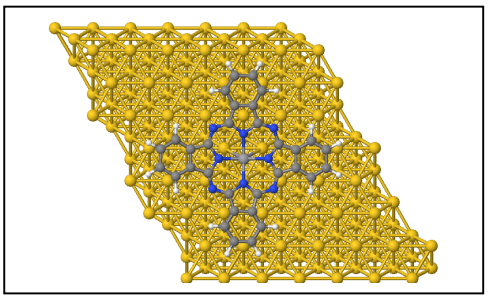

**Figure**: V-Pc on Au(111) surface/ Fcc site

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[1] G. Kresse, J. Furthmuller, *Phys. Rev. B* **54** (1996) 11169.
[2] J. Soler, E. Artacho, J.D. Gale, A. Garcia, J. Junquera, P. Ordejón, D. Sanchez-Portal, *J. Phys. Condens. Matter* **14** (2002) 2745.