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Magnetic Properties of Cobalt Monolayer between Graphene Sheets - A First-principles Study

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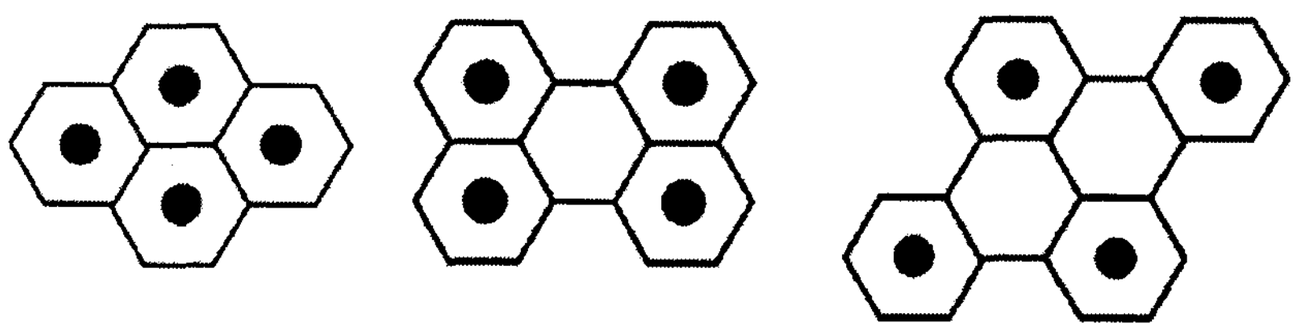
Two-dimensional (2D) magnetism in transition metal (TM) monolayers deposited on non-magnetic substrates (Ag, Au) was predicted theoreticallyfifteen years ago [1]. However, because of a possible diffusion of TM atoms into the noble material surface the results were not confirmed experimentally. Therefore, in order to obtain TM magnetic layers exhibiting 2D magnetism it is better to use graphite as an inert substrate. Homogenous monolayers (ML) of 4d transition metals were proved to grow pseudomorphically on C(0001) surface [2] and they demonstrated spontaneous 2D ferromagnetism. Providing theoretical verification of those findings, Chen et al. using a full-potential ab initio method came to a conclusion that the magnetic moment (MM) of TM atoms depended both on the ML structure and the interlayer TM-graphite distance [3].

Recently, a novel type of layered TM-graphite compound has been investigated as a material exhibiting 2D magnetic properties. In such a compound TM layers are sandwiched between adjacent graphene sheets [4]. They are expected to behave like quasi-2D magnets, and it is supposed the magnetism is similar to that of TM ML adsorbed on C(0001). Although some reports on the properties of 4d-TM monolayers on graphite surface are available, little is known about the magnetic properties of respective 3d-TM systems.

In this paper we present and discuss the results of a first-principles study of the magnetic properties of differently structured cobalt monolayers between graphene sheets.

Following the reports on investigation of the electronic and magnetic properties of 4d TM monolayers adsorbed on C (0001) surface [3] we defined the geometry of the investigated C/Co/C systems as it is shown in Figure 1.



Structure 1 Structure 2 Structure 3

The systems were simulated by a symmetrical three-layer slab with two free C(0001) surfaces and Co ML between them. Co atoms resided at hollow positions. We performed the total energy calculations in order to find the equilibrium interlayer distance in each of the structures. All the

calculationswere carried out with the use of full-potential linearized augumented palne wave method as embodied in QMD-FLAPW code [5], within generalized-gradient approximation [6].

First, the magnetic properties of the free-standing Co ML were derived. We found that magnetic moments on Co atoms in Structures 1, 2, and 3 are 2.02, 2.38, and 2.63 $_B$, respectively. It is seen that the magnitude of MM is getting larger with the extending the distance between Co atoms in the monolayer.

In the next stage, we investigated the properties of Co ML when it was resided between graphene sheets. In the all investigated structures, the value of MM on Co atom was reduced and it was 0.78, 1.18, and 0.98 $_B$ for Structures 1, 2, and 3, respectively. Although the interaction between Co ML and C(0001) sheets are rather weak, the presence of graphene sheets prevents the charge flow from Co atoms into interstitial regions. Therefore, the charge that was spread out into vacuum region in free standing Co MLs tends to occupy the available d states of Co atoms, which causes that the MM is reduced.

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