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Magnetic properties of single 3d-transition metal atom add on Born-Nitride two-dimensional array

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Abstract

In the frame work of relativistic density functional theory, using full potential local orbital band structure scheme (FPLO), the magnetic properties of single 3d transition metals (3d-TM) adsorbed on 2D hexagonal boron nitride (2D h-BN) are investigated. Binding energies between 3d-TM adatoms and 2D h-BN in three different compositions, local spin magnetic moments of 3d-TM and total spin magnetic moments per supercell, orbital magnetic moments and spin orbit coupling energies are calculated. In this study, three different magnetic relativistic methods the so-called scalar relativistic (SR), full relativistic (FR) and full relativistic plus an orbital polarization correction (OPC) are used. Results of nonmagnetic binding energies in the nonmagnetic SR method indicate that with the exception of Sc other 3d-TM adatoms can bind to BN surface. While, the results of magnetic binding energies in the spin-polarized SR approach show that Sc, Cr and Mn cannot bind on the surface of 2D h-BN. In addition, there is shown that the behavior of spin magnetic moments of 3d-TM adatoms are depended on their geometric positions due to their different crystal fields. Moreover, it is shown that Co in the top of N atoms and Fe adatoms in the top of B atoms with 1.23 (1.92) μ_Band 0.89 (1.72) μ_B have a large orbital magnetic moments in the FR(OPC) approaches due to their massive spin-orbit coupling effects, respectively. These so large values of orbital magnetic moments are promising the existence of large magnetic anisotropy energies.

Keywords: orbital magnetism, spin-orbit coupling, relativistic density functional theory

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