Induced Magnetism and Giant Perpendicular Magnetic Anisotropy of Transition Metal Doped Topological Insulator Bi(111)

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Exploring magnetism and perpendicular magnetic anisotropy (PMA) in otherwise nonmagnetic two-dimensional structures such as graphene is at the heart of spintronics research. In this talk, we will present the results of our first-principles electronic structure calculations on the possibility of reaching an atomic-scale PMA by carefully exploring the large spin-orbit coupling, orbital magnetism, and ligand field in a suitable choice of a two-dimensional structure of topological insulator Bi(111) with the Fe-, Ni-, and Co-group 3*d*, 4*d*, and 5*d* transition metal adatoms. It is identified that the substitutions of Fe, Ru, and Os transition metals in a single-layer Bi(111) have induced magnetic moments of 2.91, 0.71, and 0.65 μ_B, respectively, while the other Ni- and Co-group elements have no net magnetism. More importantly, we found the PMA energies up to an order of 100 meV per atom in Ru and Os substituted Bi(111). The underlying mechanism for the induced magnetism and large PMA will be discussed in terms of electronic structure analyses and ligand field theory.