Manipulation of magnetic anisotropy in Ir_{n+1} clusters by Co atom

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HIGHLIGHTS

- The Ir_2, Ir_4, and CoIr system possess large magnetic anisotropy energy (MAE).
- The MAE of Ir_{n+1} cluster can be manipulated by Co atom.
- Such tunable MAE is ascribed to the change in the distribution of Ir-5d orbitals.

ARTICLE INFO

ABSTRACT

Based on the first principles calculations, we have investigated the magnetic properties of Ir_{n+1} clusters modulated by Co atoms. The research conclusions show that the amplitude of magnetic anisotropy energy (MAE) and magnetization direction of the small Ir_{n+1} can be manipulated by Co atom if we can control the size very precisely. Such regulatory mechanism of MAE is ascribed to the distributing variation of Ir-5d orbits around the Fermi level induced by Co atom. More importantly, the colossal MAE values, 67.4 meV/atom, 40.26 meV/atom and 91.37 meV/atom, can be obtained for Ir_2, Ir_4, and CoIr clusters, respectively. Such high values provide a promising avenue for developing high-density magnetic storage units at sub-nanometer size.

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Minimizing the size of magnetic domain is of great interest for developing high-density spintronic data storage devices [1–3]. Nevertheless, the key issue is how to increase magnetic anisotropy energy (MAE) per atom to prevent the loss of information [4–6]. It is well known that the strong spin–orbit coupling (SOC) will lead to large MAE. In addition, the MAE is also dependent on the dimensionality and symmetry of system. For instance, for the nanostructures (e.g. clusters), due to reduced dimensionality, the spin and orbital magnetic moments are enhanced over their bulk values, thereby causing a greatly enhanced MAE. Many previous investigations have verified that the MAE of transition metal (TM) clusters [7–11] is far larger than their corresponding values in bulks. Especially, the latest 5d-TM clusters may be appropriate candidates to generate very large MAE due to strong SOC effects [12–17].

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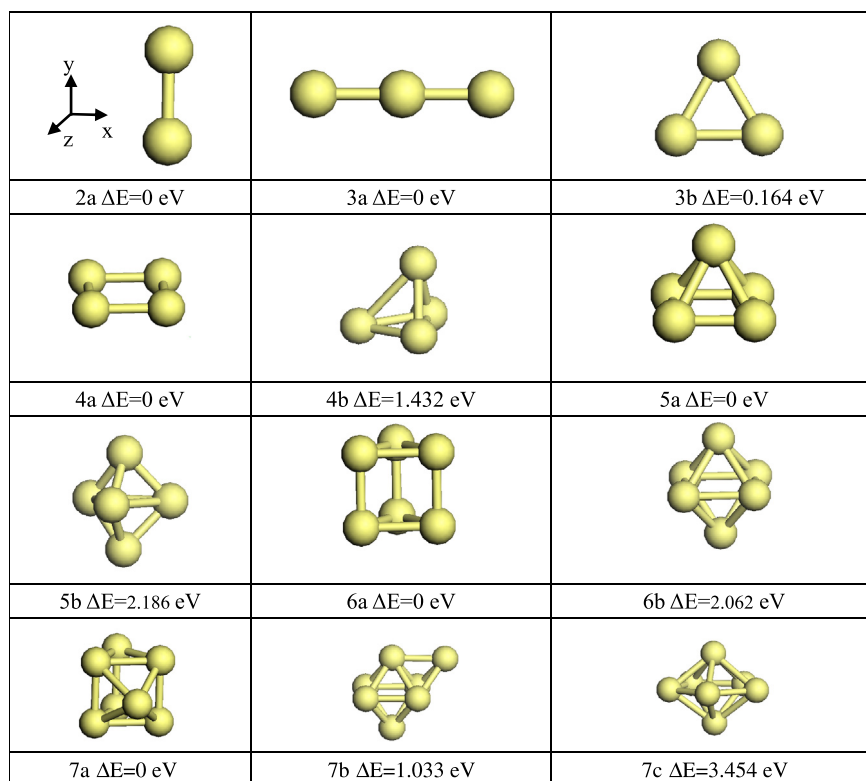*E-mail address:* wanjg@nju.edu.cn (J.-G. Wan).

Fig. 1. (Color online) The lowest energy structures of Ir_{n+1} clusters. The numbers below structure represent the differences in total energy (ΔE) between isomer and corresponding ground state structure (eV).

Although the latest mono-metallic 5d-TM clusters exhibit large MAE comparing with their bulks, the value of MAE is much lower than 1 eV which is needed for long-term magnetic storage at room temperature [18]. To further improve the temperature of long-term magnetic storage, it is necessary to design clusters with large MAE. As compared with the latest mono-metallic 5d-TM clusters, the mixed clusters of 3d-TM and 5d-TM atoms increase the possibility of designing new nano-materials with large MAE, owing to the combination of strong SOC, large magnetic moment and low symmetry [4,19–21]. Previous studies on the MAE of bimetallic clusters mainly focused on the Fe–Pt clusters [4,21], Co–Pt clusters [4,19,22], Ni–Pt clusters [4], Co–Au clusters [21], and so on. Few investigations involve the MAE of Ir-doped bimetallic clusters. Since Ir atom has the markedly SOC effect and Co has the largest MAE among 3d ferromagnetic elements [4], we expect that doping Co into Ir host clusters may be an available avenue to design novel materials with large MAE.

In this work, based on the first principles calculations, we demonstrate that the dopant Co regulates not only the magnitude of MAE but also the easy magnetization direction of host clusters. The colossal MAE values, 67.4 meV/atom, 40.26 meV/atom and 91.37 meV/atom, can be obtained, respectively, for Ir_2, Ir_4, and CoIr clusters, such high values provide a promising avenue for developing high-density magnetic storage units. We also give an insight about the origin of such tunable MAE manipulated by Co atom. We reveal that the distribution of Ir-5d orbitals around the Fermi level in the regulation of Co atom plays an important role in determining the magnetic properties of such system.

The first-principles calculations were performed in the framework of spin-polarized density functional theory (DFT) using the Vienna ab initio simulation package (VASP) [23]. Nonlocal exchange correlation energies were treated with Perdew–Burke–Ernzerhof (PBE) [24] functional based on the generalized gradient approximation (GGA). Plane waves [25,26] with energy cut-off of 500 eV were used for the expansion of Kohn–Sham orbitals. The equilibrium geometries were obtained when the atomic forces were smaller than 0.010 eV/Å. The MAE value was estimated by implementing SOC in VASP in a noncollinear mode [27]. During the calculation of MAE, the geometric, electronic, and magnetic degrees of freedom were relaxed simultaneously until the change in total energy between successive iteration steps were smaller than 10^{-7} eV. All calculations were performed with a cubic box of 15 Å and using a single **k** point (Γ point) for the Brillouin-zone integration. As for the initial magnetization orientation, we chose y axis perpendicular to the basal plane or parallel to the axis of dimer (trimer), x and z axes are in the basal plane or perpendicular to the axis of dimer (trimer), as shown in Figs. 1 and 2. E_x, E_y and E_z are the total energies of cluster along x, y and z magnetization directions, respectively.

To test the accuracy of computational methods, the Ir_2 dimer was calculated. The calculated bond length and binding energy are 2.210 Å and 2.313 eV/atom, respectively. The calculated bond length is consistent with the theoretical data of 2.247 Å–2.287 Å [28–33], and moreover, these values are also agreement with experimental data of 2.230 Å, 2.350 Å, 2.250 Å