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Magnetism of Zr atomic wires*

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By using the full-potential linearized augmented plane wave method to perform *ab initio* total energy calculations, we have explored magnetic ordering in one-dimensional Zr wires. The result shows that Zr can form linear, or dimerized, or zigzag wires, and the magnetic properties strongly depend on their geometric structures. The linear and zigzag wires exhibit ferromagnetic ground states at the equilibrium bonding distance, while the dimerized wire, despite its higher stability than that of the linear one, exhibits nonmagnetic ground states. The most stable geometry is shown to be the zigzag wire with a magnetic moment of 0.26 μ_B per atom.

Keywords: magnetism, Zr atomic wire, *ab initio* calculations
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1. Introduction

During the last two decades, rapid advances in magnetic overlay and multilayer systems have led to the discovery of a number of fundamental physical phenomena such as dimensionality-induced magnetization of nonmagnetic metals, oscillatory magnetic coupling, and giant magnetoresistance.[1] With current experimental techniques, nano-structured systems with desired dimensionality can be achieved in a well-controlled manner, which allows a study of the influence of dimensionality on material properties in great detail. Novel magnetic properties at reduced dimensionality are of particular interest. In this aspect, there are only limited theoretical studies and whether magnetic ordering exists in such a system is still somewhat controversial. Recent first-principle calculations[2−4] reported the magnetic ordering for Al and Ga nanowires. Shen *et al*[5] studied the electronic structure and stability of Nb atomic chains. Spišák and Hafner[4] performed first-principles studies on the wires composed of the fifth and sixth row elements in the periodic table with the pseudopotential–plane-wave (PPPW) method and predicted the magnetism for the early transition metals Zr and Ta. More recently, Lin *et al*[6] studied the atomic and electronic structures of Zr atomic chains with the *ab initio* pseudopotential approach and found that Zr could form planar chains in the forms of zigzag, dimer and ladder structures. However, information on magnetic properties of Zr wires is missing. The present work is devoted to the magnetic properties of the Zr monatomic wires.

We systematically investigate the total energy, electronic and magnetic properties of Zr wires by using the full-potential linearized augmented plane wave (FLAPW) method. Our study suggests that the linear and zigzag wires exhibit magnetic ordering at the equilibrium bonding distance, while the dimerized structure is nonmagnetic.

2. Computational method

All calculations are performed with WIEN2K package[7] by using the self-consistent FLAPW method under the generalized gradient approximation (GGA).[8] The FLAPW is considered to be the most accurate method of predicting electronic structures and magnetic properties. In the FLAPW method, no shape approximation is made in charge, potential, and wave-function expansions. The valence electrons are treated in a scalar-relativistic approximation, while core states are treated fully relativistically in an atomic-like approximation. In the present work, three possible geometries of Zr wires are considered, as shown in Fig.1. A supercell is constructed for sim-

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ulation of the isolated Zr wires. The distance between the atomic wires is taken as 1.6nm, which is sufficient to eliminate the inter-wire interactions. The supercell size is set as XYZ=1.6nm $\times$1.6nm $\times Z$nm, in which the value in the Z-direction varies with bond length and structural type of the wires. The muffin-tin (MT) radius for Zr is 0.1164nm. Spherical harmonics with a maximum angular quantum number of 10 is used to expand the charge, potential and wave functions in the muffin-tin sphere. The cut-off parameter is $R_{\rm mt}K_{\rm max} = 5.0$ for the plane wave expansions in the interstitial region. The Brillouin zone sampling is performed using 64 special-k-point meshes, which yields 15 points in the irreducible Brillouin zone. With these optimized parameters, the total energies can be converged within 1meV.

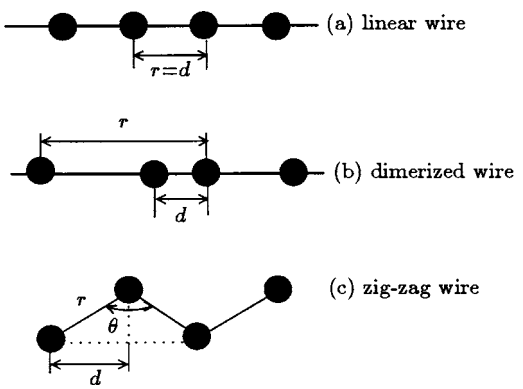


Fig.1. Illustration of the geometry of the linear, dimerized, and zigzag wires.

3. Results and discussion

First of all, we study the magnetic property of the linear chain. The spin-polarized calculation indicates that magnetic configurations in the linear wire have a lowest total energy. In Fig.2, we show the total energies of the linear Zr structure as a function of interatomic distance in the paramagnetic (PM), ferromagnetic (FM) and antiferromagnetic (AFM) states. It is clear that the ferromagnetic state is energetically most favourable. Minimization of the total energy with respect to interatomic distance gives an equilibrium bond length of r=0.254nm and a magnetic moment of 0.45$\mu_{\rm B}$/atom, which are comparable with 0.255nm and 0.38$\mu_{\rm B}$/atom by Spišák and Hafner.[4] On the other hand, the AFM state is 18meV/atom higher in energy than that of the FM one, with an alternative magnetic moment of 0.41$\mu_{\rm B}$/atom. In the PM calculation, the energy is 27meV higher than that of the FM state at the equilibrium bond distance.

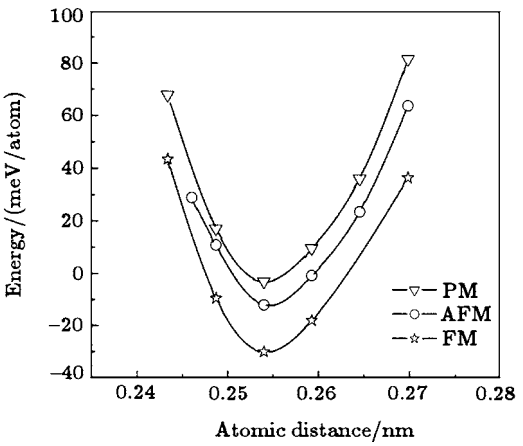


Fig.2. Relative total energies of the linear wire for different magnetic configurations as a function of interatomic distance (r).

For the dimerized wire shown in Fig.1, the distance r between the second nearest neighboring atoms maintains a constant of 0.543nm as reported by Lin *et al*,[6] but the atom in the middle of a cell moves along the wire. It is rather surprising that no magnetism is found at the equilibrium bond length for the dimerized wire, and both FM and AFM calculations show zero magnetic moment and have the same total energy as that of the nonmagnetic (NM) one. However, the dimerized wire is more stable than the linear wire. Minimization of its total energy results in a dimer bond distance of d=0.234nm which is consistent with 0.233nm by Lin *et al.*[6]

In the calculation of the zigzag wires, the nearest-neighbour distance r maintains a constant of 0.274nm which is the same as the optimized result in previous work,[6] while we optimize the zigzag angle θ. It is interesting that magnetic ordering is found again in this structure, and the spin-polarized total energy calculations give an equilibrium angle of θ =63° with a magnetic moment of 0.26$\mu_{\rm B}$/atom. The AFM configuration exhibits a magnetic moment of 0.23$\mu_{\rm B}$/atom, 12meV/atom higher than that of the FM ground state in energy. While the PM state is 20meV higher than that of the FM one as shown in Table 1.

Table 1. Calculated equilibrium geometry parameters, magnetic moment (μ_B/atom) and energy difference ΔE (eV/atom) with respect to NM state of the linear wire.

Structure				FM		AFM		NM
	r/nm	d/nm	θ/(°)	m/μ_B	ΔE/eV	m/μ_B	ΔE/eV	ΔE/eV
Linear wire	0.254	0.254	180	0.45	–0.027	0.41	–0.009	0
Dimerized wire	0.543	0.234	180	–	–	–	–	–0.121
Zig-zag wire	0.274	0.143	63	0.26	–1.248	0.23	–1.236	–1.228

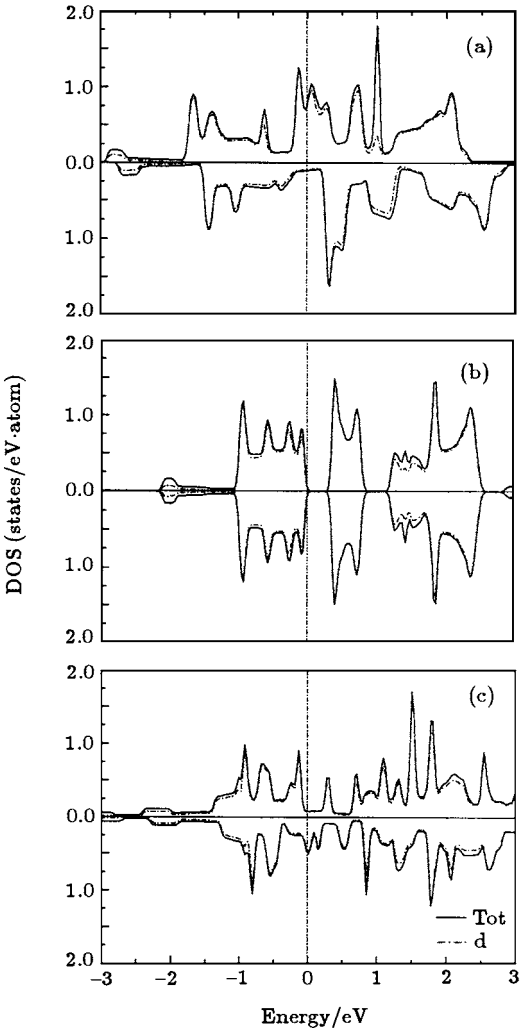


Fig.3. Spin-dependent total (Tot) and partial densities of states (DOS) of the Zr wires: (a) the linear wire in FM state, (b) the dimerized wire, (c) the zigzag wire with a bond-bond angle of 63° in FM state. The zero energy is set at Fermi level (denoted by the vertical dotted lines).

To understand the origin of magnetic properties, the spin-dependent total and partial densities of states (DOS) with respective equilibrium bond lengths for different geometries are studied and displayed in Fig.3. The DOS for the magnetic state in either the linear or zigzag structure is obvious, as seen in Fig.3(a) and (c), respectively. There is a split between spin-up and spin-down in the total DOS, which induces magnetic ordering in both structures. From the partial electronic DOS, one can see that the DOS near the Fermi level is mainly from 4d electrons, with a negligible contribution from the s and p electrons. The DOS for the dimerized wire with nonmagnetic states is shown in Fig.3(b). It shows that the electronic densities of spin-up and spin-down states with an energy gap being about 0.4eV are equally occupied, which leads the dimerized structure to have nonmagnetic ground states.

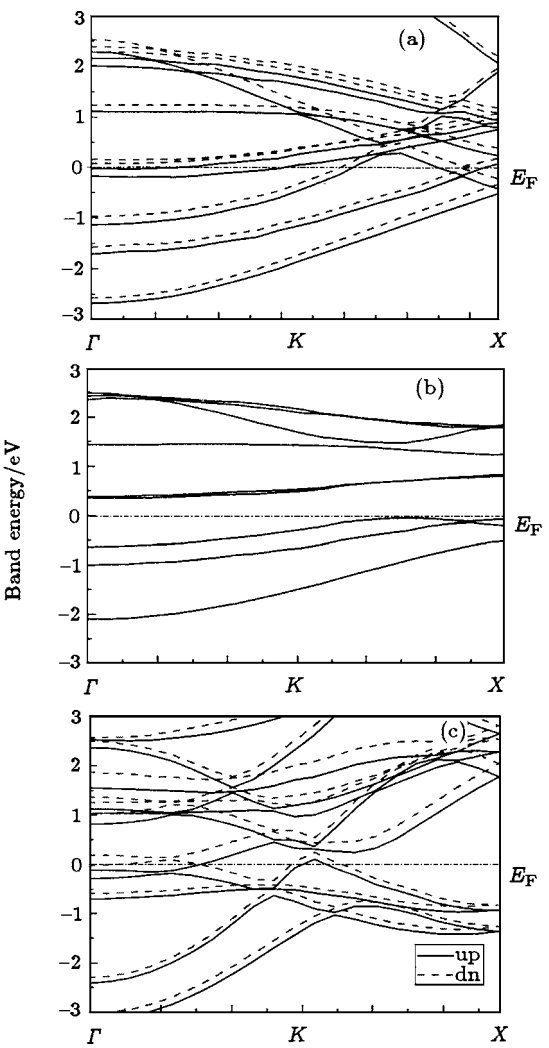


Fig.4. Band structures of the Zr wires. (a) The linear wire in FM state; (b) the dimerized wire with NM state; (c) the zigzag wire with a bond–bond angle of 63° in FM state. The solid (dashed) lines depict the up (down) spin states. The zero energy is set at Fermi level (E_F).

In order to provide a further insight into the electronic structure and magnetic properties of the Zr wires, we show the calculated electronic band structures in Fig.4. One can see that the band structures near the Fermi level undergo significant changes in different structures. The splitting of the bands due to the magnetic ground state occurs in the linear and zigzag wires, which does not occur in the dimerized wire. On the other hand, in spite of the difference in band structure, there exists a metallic character in both linear and zigzag structures. For the dimerized wire with the nonmagnetic states, there exists an energy gap being $\sim$0.4eV at Γ point.

4. Conclusion

In summary, the electronic structures and possibilities of magnetic ordering in one-dimensional Zr wires are studied with the FLAPW method. The results reveal that the magnetic properties depend strongly on the geometric structure. The straight linear and zigzag wires show magnetic ordering at the equilibrium bond length and the FM configuration having lower energy than both PM and AFM ones. All magnetic states have a typical magnetic moment 0.2–0.5$\mu_{\rm B}$/atom. To understand the magnetic properties, the density of states and band structures are also studied. We expect this study to be capable of stimulating some experimental efforts to explore the magnetism of nanowires of elements that are nonmagnetic in its bulk form. This kind of wire can be prepared by using anisotropic metal or semiconductor substrate, such as Co/ Pt(997).[9]

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