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# Magnetism and electronic structure of Fe chains and nano-wires

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**Abstract**

The electronic and magnetic structures of an Fe linear chain and FCC and BCC nano-wires were determined by accurate first-principles self-consistent full potential linearized augmented plane wave calculations. The one-dimensional nature of the systems results in dramatic changes in their properties—as expected from the early predictions of Weinert and Freeman (J. Mag. Magn. Mater. 38 (1983) 23) for linear transition metal chains: a high density of states arising from van Hove singularities, large s–d-exchange splittings (larger in the chain than in the wires) and filled majority d bands (i.e., a "strong Stoner" ferromagnet) and strikingly enhanced Fe magnetic moments that depend on their coordination number. These unusual and distinctive properties are expected to invite somewhat unique experimental characterizations.


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Nanostructured magnetic materials involving transition metals are now a subject of very active research both theoretically and experimentally. Magnetism in one-dimensional systems has been emphasized since the work of Ising [1] and treated with very simple qualitative models or semi-quantitative numerical approaches, until the pioneering work of Weinert and Freeman exactly 20 years ago. These authors [2] carried out accurate self-consistent local spin density full-potential linearized augmented plane wave (FLAPW) calculations [3] for linear chains of Ni and Fe atoms which realistically treated their 3D nature for the first time. Some rather unusual properties were predicted with distinctive features that make their experimental characterization feasible.

Recently, interest in 1D-like systems has centered on transition metal chains and wires [4,5] and sophisticated experiments (including MCD—magnetic circular dichroism) and calculations (including magnetic anisotropy energy [6]) have been performed. In this paper, we report briefly on the electronic structure and magnetism of Fe linear chains and wires as calculated using the FLAPW method based on density functional theory within both the local density approximation (LDA) and generalized gradient approximation (GGA). We also employ MCD calculations [7] based on the FLAPW results to assess the absorption spectra and magnetic moments. We focus on the effects of the local environment on the electronic structure and spin magnetic moments for the Fe chain in comparison with results for the Fe wires.

We consider three free-standing systems: (i) an Fe atomic chain, (ii) an FCC Fe nano-wire and (iii) a BCC Fe nano-wire. For the FCC (BCC) wire, we take the FCC (BCC) unit cell and extend it along the (0 1 0) direction to form an infinite nano-wire as shown schematically in Fig. 1.

All calculations are performed with the thin film version of the FLAPW method [3]. The lattice constant of the Fe chain is chosen as the nearest-neighbor

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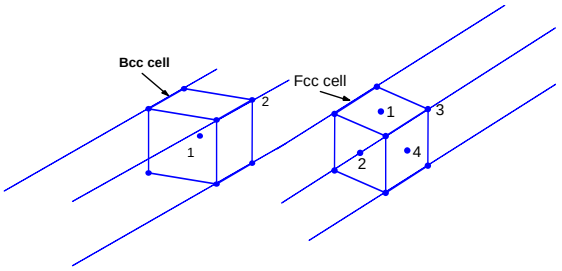


Fig. 1. Structure and numbering of Fe sites in the FCC and BCC nano-wires.

distance $a = 2.486$ Å in bulk BCC iron and the lattice constant of the BCC and FCC nano-wires is chosen as $a = 2.87$ and 3.61 Å, respectively.

The spacing between chains (wires) in the supercell method are taken to be $4a$ ($3a$). An energy cut off of 12.25 Ry is used for the variational plane wave basis set, and the muffin-tin radius is taken to be 2.30 a.u. for all three systems. Within the muffin-tin spheres, lattice harmonics with maximum angular momentum $l_{max} = 8$ are employed to expand the charge density, potential and wave functions. Convergence is assumed when the average root-square distance between the input and output charge and spin densities is less than $10^{-4}$ e/(a.u.)$^3$. In the self-consistency procedure, the number of k-points is taken as 24 for the BCC wire and 30 for the FCC wire. Starting from the converged ground state, the spin–orbit coupling (SOC) is treated in a second variation to obtain the electronic structure and MCD absorption spectra.

As found previously [2] for the Fe linear chain, there is a large s–d interaction, the majority d-bands are filled (as in a strong Stoner ferromagnet), and van Hove singularities (infinities) in the density of states (DOS) which has a gap between majority and minority spin bands below $E_F$. This gap exists whether the GGA or the LDA (von-Barth–Hedin) exchange-correlation is used. But there is no gap between majority and minority spin bands for the BCC and FCC Fe nano-wires. Clearly, the s–d exchange interaction for the chain is stronger than that for the wire. For the three systems, the DOS at $E_F$ is predominantly occupied by d states: spin-down states from the d-band of the Fe(2) atomic site strongly dominate at $E_F$ because Fe(2) is on the edge of the BCC wire.

The calculated magnetic spin moments are found to be dramatically enhanced from that of bulk Fe (2.15 $\mu_B$/atom) and should result in enhanced hyperfine interactions and other properties. This reflects the effect of reduced coordination number of each atomic site inside the chain and BCC and FCC wires. The Fe chain moment is 3.30 $\mu_B$/atom and the spin magnetic moment of Fe(1), Fe(2), Fe(3) and Fe(4) sites in FCC wire is 2.85, 2.69, 3.03 and 2.86 $\mu_B$/atom, respectively. The largest magnetic moment is from the atom on the edge, the next largest from the atom on the face, and the smallest from the atom inside the wire—again indicating that the spin magnetic moments become larger for reduced coordination numbers. This behavior is also found in the BCC wire. The spin magnetic moment of Fe(1) and Fe(2) sites in the BCC wire is 2.42 and 3.11 $\mu_B$/atom, respectively. Again, as expected, the local environment of the Fe atom plays an important role in the magnetic moment of the same wire.

From the calculated MCD absorption cross-sections (not shown), we find that the average spin magnetic moments of the Fe chain, BCC wire and FCC wire are 3.30, 3.02 and 3.06 $\mu_B$/atom, respectively, as expected, since the lowered dimensionality results in larger magnetic moments. Similarly, the orbital magnetic moments are, of course, also enhanced and will be presented elsewhere.

We have described briefly a number of results obtained for these linear systems, including dramatically enhanced magnetic moments that clearly reflect the reduced dimensionality and reduced coordination number. They serve to emphasize the unique aspects of magnetism at the nanoscale and invite further study with newly developed sophisticated experimental techniques.

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