Band Structure Engineering of Si [110] Nanowire by Surface Passivation and Wire Diameter Control

Zhi-Ren Xiao, Li-Ger Chen and Guang-Yu Guo

In this research, we investigate how the different types of surface-passivated atom or various kinds of wire radii affect on the characters in the band structure, such as the band gap and effective mass for electrons or holes, of Si nanowires.

Our research method is theoretical calculation based on local density approximation (LDA) density functional theory, as implemented by *OpenMX* code. The program uses norm-conserving pseudo-potential and solves the electronic states by *O*(*N*) Krylov-subspace method. The basis is using LCAO with optimized orbitals. During the geometrical relaxation calculation, the *s2p2d1* basis for Si and F and the *s2p2* basis for H are contracted to *s1p1* basis for increasing the efficiency for large scale calculation. We use eigenvector following (EF) method to find the stable geometry of the nanowires, but we fix the length of the wires (1.92Å/ML along wire direction) to ignore the stress effect. The k-points in SCF calculation are set as 1×1×6 for geometrical optimization and 1x1x32 for band structure plotting.

The electronic structures and band gaps of Si nanowires in [110] direction are studied by simulating the slabs with periodic boundaries on [110] facets (shown in Fig 1). Combining the genetic algorithm (GA) with *ab initio* calculation, Chan *et al.* have found the hexagon section structures are stable when the diameters are between 1.3nm to 7.0nm.

In this research, our slabs for nanowire are the hexagon sections, and diameters of the wires from ring1 to ring 5 are 3.84Å, 11.52 Å, 19.20 Å, 26.88 Å and 34.56 Å, respectively. Both two types of wire surface passivation (H and F) are investigated to understand how the passivation affects the band gaps. In order to avoid the H-H or F-F interactions on the wire surface, we apply the twist for H-Si-H or F-Si-F trimers on [100] facets then find out the stable geometry by structural relaxation.

The band gaps versus the radius for H- and F-passivated Si nanowires are shown in Fig 2. Previous theoretical calculations for other halogens (Cl, Br and I) passivation nanowires show red shift of the band gap comparing to hydrogen-passivated wires. In our cases the fluorine passivation also induces red shift of the band gap

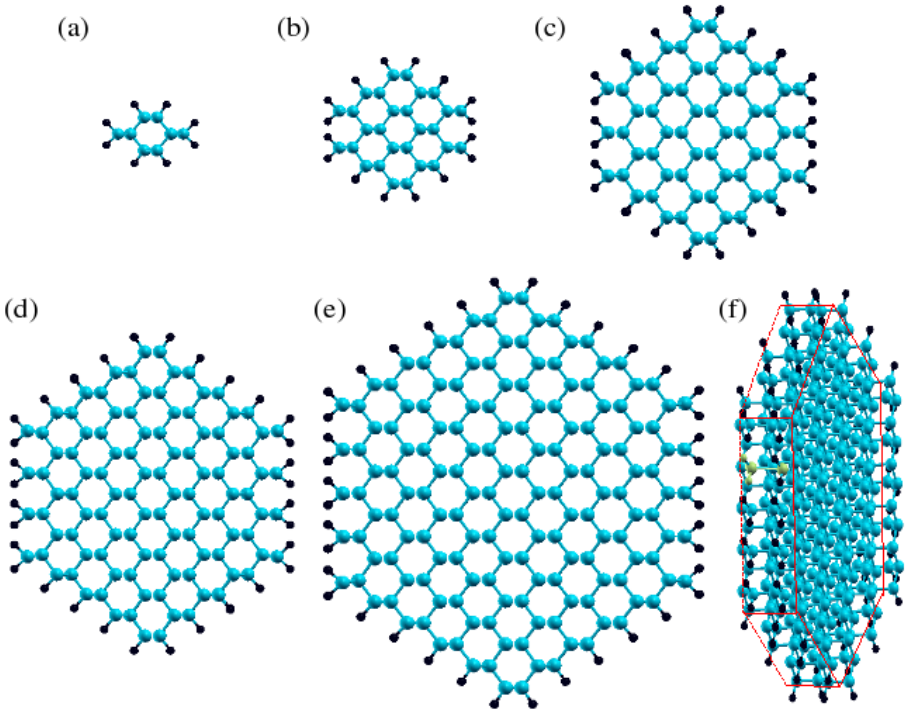


Fig 1: The Si [110] nanowire. The radius of the (a) ring 1, (b) ring 2, (c) ring 3, (d) ring4 and (e) ring 5 are 1.92Å, 5.76 Å, 9.60 Å, 13.44 Å and 17.28 Å, respectively. The blue sphere represents Si atom, while the black sphere represents H or F atom. Figure (f) shows the unit slab for ring 5 in calculation. On [100] facet, the green spheres shows the twist between the F-Si-F trimer and Si-Si bond along wire direction.

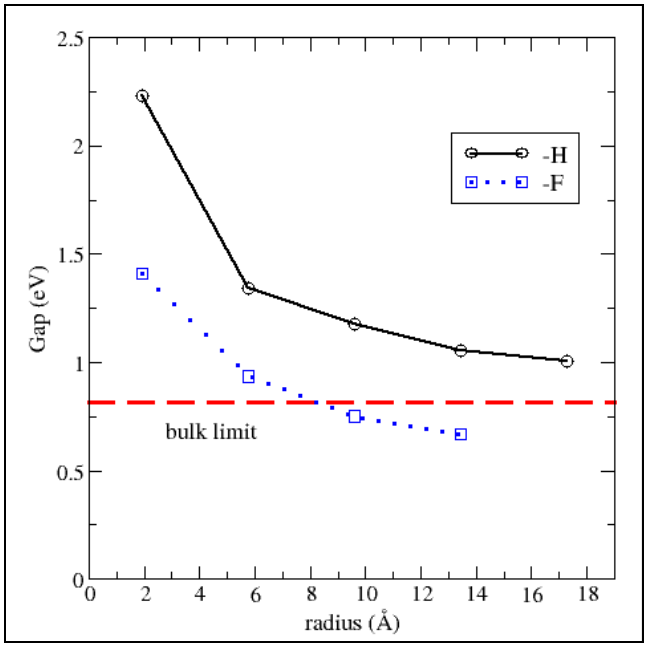


Fig 2: The band gap changes with the wire diameter and surface passivation for the Si [110] nanowire.

Ab initio study of possible superconductivity in n-type InN

Shao-Hua Chen and Guang-Yu Guo

Traditionally, we distinguish materials as conductor, semiconductor, and insulator by its conductivity. We know conventional superconductor (< 40k, not high temperature superconductor) is metals or alloys. The possibility of superconductivity in semiconductors has been discussed long ago. It had been observed superconducting properties in doped semiconductors in recent years.

From BCS theory, We know the central idea is Cooper pair's mechanism. It is possible to compute the electron-phonon coupling from first principle. Dacorogna and Cohen had been developed a new approach to calculate electron-phonon coupling in metals in 1985. Savrasov et al had obtained superconducting properties in many elemental metals by ab initio linear-response calculations. Some others ab initio theoretical study of doped semiconductors given consistently results of superconducting properties with experiments .

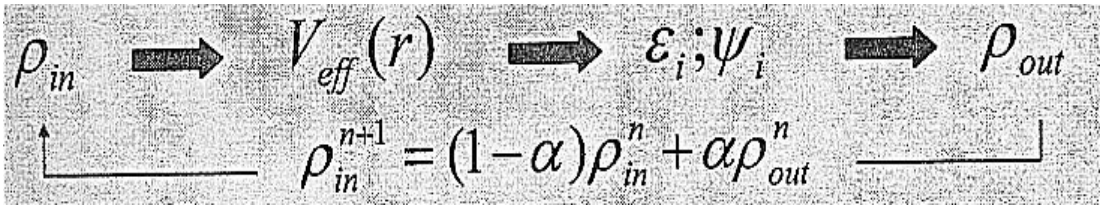
InN is a III-nitride semiconductor, play important role for optical device. It is hexagonal, wurtzite structure under ambient enviroment. In this research we presented an ab initio study of superconducting properties of the n-type InN and compare to the results of experiments. The reasearch is still going on.

What is First principle(*ab initio*)

By solving the SchrÖdinger equation that describes the motion of the electrons in the Coulomb potentials of the nuclei and of each.

By first-principles *(ab initio*), we mean empiral parameter-free calculations; that is, calculations in which the only input is the atomic numbers, species,structure and potential of the atoms .

Self-consistent itrative calculation



Some calculation parameters

Code :Pwscf (Plane-Wave Self-Consistent Field) package –Quantum Espresso-3.2

http://www.pwscf.org

PseudoPotentials :

In.pz-bhs.UPF

N.pz-vbc.UPF

Sn.pz-bhs.UPF

Cut off energy of eigenstates : 30 Ryd

Cut off energy of charge density : 120 Ryd

K-points : 10x10x8 Monkhorst-pack grid

q-points : 5x 5x4 Monkhorst-pack grid

doped (%)	lambda	Cal Tc	Exp Tc
0.01	~0.09	~0	~0.12
0.1	~0.09	~0	~1
1	0.45	~0.09	2~3
10	0.56	1.43	2~3

Table , different doped percentage of n-type InN and its electron-phonon coupling constant (lambda) , calculated superconducting transition temperature (Tc) ,experimented value .

Systematic Ab initio study of electronic and magnetic properties of 3d transition metals linear and zigzag chain

Jen-Chuan Tung and Guang-Yu Guo

Magnetism at the nanometer scale has been a very active research area in recent years, because of its novel fundamental physics and exciting potential applications. Theoretically, a great deal of research has been done on both finite and infinite chains of atoms. In particular, calculations for isotropic Heisenberg model with finite-range exchange interactions show that a one dimensional (1D) chain cannot maintain ferromagnetism at any finite temperatures. Nonetheless, this discouraging conclusion has to be revised when a magnetic anisotropy is present, as in, e.g., quasi-1D crystals. Experimentally, modern methods to prepare nanostructured systems have made it possible to investigate the influence of dimensionality on the magnetic properties. A fundamental idea is to exploit the geometrical restriction imposed by an array of parallel steps on a vicinal surface along which the deposited material can nucleate. For example, Gambardella, et al., recently succeeded in preparing a high density of parallel atomic chains along steps a high density of parallel atomic chains along steps and also observed 1D magnetism in a narrow temperature range of 10~20 K. Structurally stable nanowires can also be grown inside tubular structures, such as the Ag nanowires of micrometer lengths grown inside self-assembled organic (calix[4]hydroquinone) nanotubes. Short suspended nanowires have been produced by driving the tip of scanning tunneling microscope into contact with a metallic surface and subsequent retraction, leading to the extrusion of a limited number of atoms from either tip or substrate. Monostrand nanowires of Co and Pd have also been prepared in mechanical break junctions, and full spin-polarized conductance was observed. The monoatomic chains, being an ultimate 1D structure, are a testing ground for the theories and concepts developed earlier for three-dimensional (3D) systems.

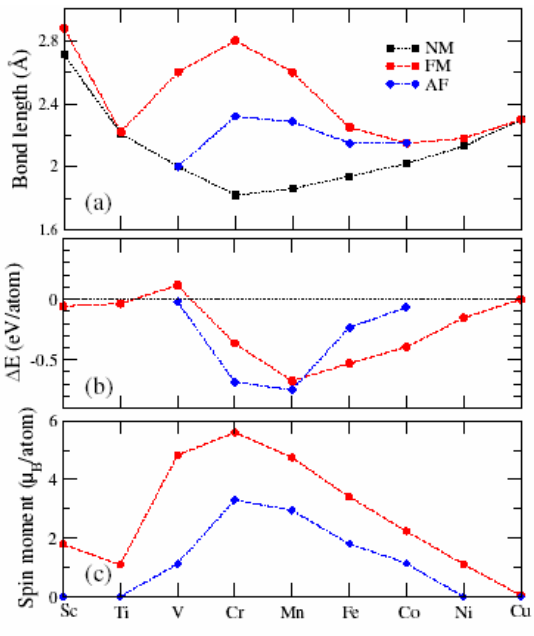
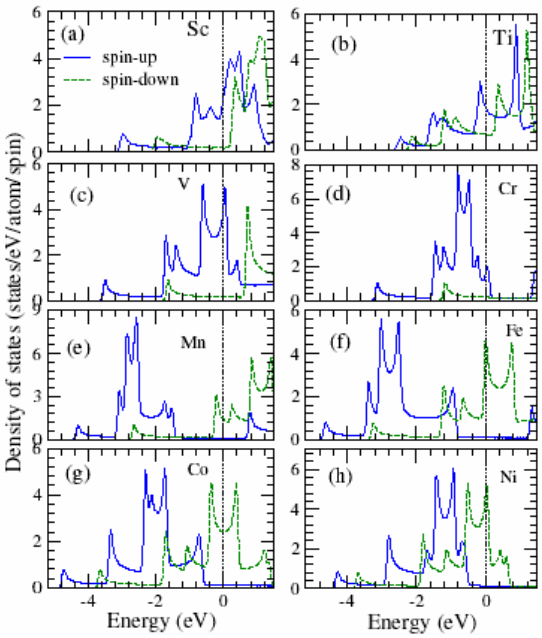


FIG. : (color online) (a) Equalibrium bond lengths, (b) magnetization energy (ΔE) (i.e., the total energy of a magnetic state relative to that of nonmagnetic state) ($\Delta E = E^{FM(AF)} - E^{NM}$) and (c) spin magnetic moments (μ_B) of all the 3*d* transition metal linear atomic chains in the NM, FM, and AF states.

Furthermore, the 1D characters of nanowires can cause several new physical phenomena to appear. It is of fundamental importance to understand the atomic structure in a truly 1D nanowire and how the magnetic and electronic properties change in the lower dimensionality. Therefore, theoretical calculations at either semi-empirical tightbinding or ab initio density functional theory level for many infinite/finite chains, e.g., linear chains of Co, Fe, Ni, Pd, Pt, Cu, Ag, and Au, as well as zigzag chains of Ti, Fe, and Au, have been reported. Early studies of infinite linear chains of Au, Al, Cu, Ca, Pd, and K have shown a wide variety of stable and metastable structures. Recently, the magnetic properties of transition metal infinite linear chains of Fe, Co, Ni, have been calculated. These calculations show that the metallic and magnetic nanowires may become important for electronic/optoelectronic devices, quantum devices, magnetic storage, nanoprobes and spintronics.



Despite of the above mentioned intensive theoretical and experimental research, current understanding on novel magnetic properties of nanowires and how magnetism affects their electronic and structural properties is still incomplete. The purpose of the present work is to make a systematic ab initio study of the magnetic, electronic and structural properties of both linear and zigzag atomic chains of all 3d transition metals (TM). Transition metals, because of their partly filled d orbitals, have a strong tendency to magnetize.

Nonetheless, only 3d transition metals (Cr, Mn, Fe, Co, and Ni) exhibit magnetism in their bulk structures. It is, therefore, of interest to investigate possible ferromagnetic (FM) and antiferromagnetic (AF) magnetization in the linear chains of all 3d transition metals including Sc and Ti which appear not to have been considered. As mentioned before, recent ab initio

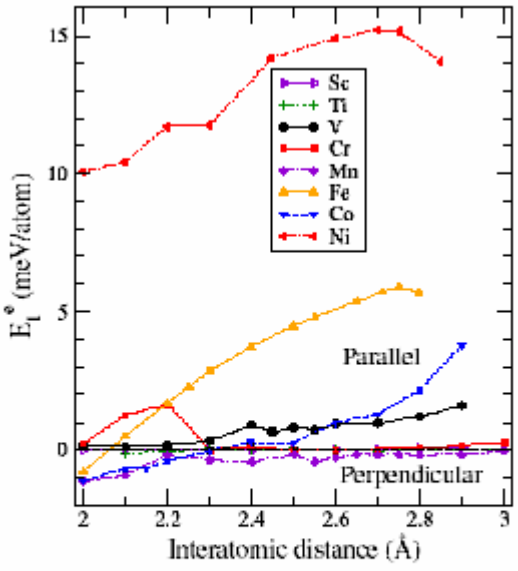


FIG. : (color online) Magnetocrystalline anisotropy energy (E_1^e) of the 3*d* transition metal linear atomic chain as a function of interatomic distance. A positive value of E_1^e means that the magnetization would be parallel to the chain axis whilst a negative value would means that the easy magnetization axis would be perpendicular to the chain.

calculations indicate that the zigzag chain structure of, at least, Ti and Fe is energetically more favorable than the linear chain structure. Thus, we also study the structural, electronic and magnetic properties of all 3d transition metal zigzag chains in order to understand how the physical properties of the monoatomic chains evolve as their structures change from the linear to zigzag chain.

Relativistic electron spin-orbit coupling (SOC) is the fundamental cause of the orbital magnetization and also the magnetocrystalline anisotropy energy (MAE) of solids. Knowledge of the MAE of nanowires is a key factor that would determine whether the nanowires have potential applications in, e.g., high-density recording and magnetic memory devices. Ab initio calculations of the MAE have been performed for mainly the Fe and Co linear chains, while semiempirical tight-binding calculations have been reported for both linear chains and two-leg ladders of Fe and Co. Unlike 4d and 5d transition metals, the SOC is weak in 3d transition metals. Nonetheless, the MAE could be very large in certain special 3d transition metal structures such as tetragonal FeCo alloys. Therefore, as an endeavor to find nanowires with a large MAE, we have calculated the MAE and also the magnetic dipolar (shape) anisotropy energy for all 3d transition metals in both the linear and zigzag structures. Indeed, we find that the FM Ni linear chain has a gigantic MAE. Although in this paper we study only free-standing 3d transition metal chains, the underlying physical trends found may also hold for monoatomic nanowires created transiently in break junctions or encapsulated inside 1D nanotubes or deposited on weakly interacting substrates, albeit, with the actual values of the physical quantities being modified.