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REGULAR ARTICLE

Modulation of the work function of silicon nanowire by chemical surface passivation: a DFT study

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Abstract The electronic structures and work functions of hydrogen (H−), fluorine (F−), and hydroxyl (OH−) passivated silicon nanowires (SiNWs) are evaluated by DFT calculations. We reveal that the work function of SiNW depends strongly on the nature of passivating functional groups, the percentage of passivation and the surface passivated. In particular, a trend of work functions: F-SiNW > H-SiNW > OH-SiNW, is obtained. Taking H-SiNW as the reference, the increased work function in F-SiNW is attributed to the electron withdrawing effect from highly electronegative F atom. In contrast, although O atom is also highly electronegative, for OH-SiNW, such effect is countered by the resonance effect in which electron is donated back to the SiNW surfaces, resulting in reduced work function. The extent of the increment or reduction is proportional to the percentage coverage of the passivating chemicals. Moreover, the work function changes more significantly when the di-substituted (100) surfaces are passivated than that of the mono-substituted (110) surfaces. Consequently, OH-SiNW shows conjugate-liked Si–Si bonds at both the surfaces and the core. The results indicate that the work function of SiNW can be fine tuned by using selected chemical on selected surface with known amount of coverage for customizing purpose.

Keywords Silicon nanowire · Work function · DFT · Surface modification

1 Introduction

Extensive experimental and theoretical works on silicon nanowires (SiNWs) have been carried out in recent years. In particular, studies include synthesis [1–5] and electronic structure calculations of SiNWs [6–15]. SiNWs have attracted much attention because of its special features such as high surface to volume ratio, one-dimensionality, biocompatibility and tunable band gap. Leveraging on such characteristics, SiNWs have recently been utilized in many device applications such as biological and chemical sensors [16, 17], field-effect-transistors [18], solar cell [19] and optoelectronics [20]. Currently, those SiNWs utilized in devices are usually coated with SiO_2. To further extend and customize its applications, surface modification of SiNWs by chemical species is one of the feasible ways to achieve it. The passivating functional groups would generally modify the electronic properties of SiNWs. An insightful understanding of such passivating functional groups induced electronic effect is thus important to understand the intrinsic properties of surface modified SiNWs.

Among the commonly measurable parameters in experiments, work function (WF) is one of the important parameters to be considered for selecting materials in device design. Work function is defined as the energy required to remove an electron from the Fermi level to the vacuum level of the material [21]. It reflects the intrinsic

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properties of the material surfaces and provides important knowledge on the reorganization of electronic charges caused by surface modifications, which directly related to its application. For examples, in thin-film optoelectronics, the work functions of the layered materials have strong influence on electron and hole transport properties; in scanning tunneling microscopy, the work function of the tip material is also crucial for the measurement.

However, as compared with other electronic properties, such as band gap examination, very limited theoretical study on the work function of SiNWs has been reported. In particular, Leu et al. [12] reported the effect of strain on the work function of H-passivated ⟨110⟩ and ⟨111⟩ SiNWs with different diameters. Their calculations showed that the work functions of the SiNWs are slightly affected by their sizes. However, for surface modified SiNWs, related theoretical work has not yet been reported so far.

In this work, we report the modulation of the work function of SiNW by chemical surface passivation using DFT calculations. Work function, the Fermi level and vacuum potential are the key properties to be discussed. We focus on determining how the size of the nanowire and the chemical properties of the surface passivating atoms would affect the work function of the SiNWs. Since the smallest SiNW observed so far has a diameter of ~1 nm [22], we adopt the SiNW models with diameters of ~1 to ~2 nm. For determining the surface effects, we select H, F and OH because F and O are both highly electronegative atoms, which should have strong effects in modulating the work function of SiNWs.

2 Methods

All calculations are done by using generalized gradient approximation (GGA) scheme (PW91) [23] within DFT implemented in Vienna Ab initio Simulation Package (VASP) [24, 25]. We use the frozen-core projector augmented wave (PAW) method to describe the interactions between ions and electrons [26]. A cutoff energy of 450 eV is used for the plane wave expansion. Default value of density cut-off chosen by the program is used. Monkhorst–Pack sampling with 1 × 1 × 8 *k*-point grid is used. *k*-point tests show that the total energy difference is less than 0.001 eV when larger k-point grids (1 × 1 × 9 and 1 × 1 × 10) are used. For the simulation cell, the nanowire is oriented parallel to the *z*-direction and the vacuum spaces are along the *x*- and *y*- directions. Two primitive unit cells along the axial direction are used for each nanowire so that the length along the *z*-direction of the cell is 7.680 Å before optimization (Fig. 1a). For geometry optimization, vacuum spaces of more than 12 Å in the lateral directions are used to avoid interactions between neighboring ions. The unit cell is only optimized in the *z*-direction. Both the ion and unit cell are fully relaxed until the absolute value of force acting on each atom is less than 0.01 eV/Å. For the work function calculations (we refer the readers to our previous works [27]), the average vacuum potentials for each nanowire are determined by single-point energy calculations.

For the charge density analysis, we calculate the charge density difference (CDD) between the passivating atoms and the SiNW using the formula: $CDD = CD_{X\text{-}SiNW} - CD_X - CD_{SiNW}$ where CD_{X-SiNW}, CD_X and CD_{SiNW} are the charge densities of the X-SiNW (X = H, F, or OH), the passivating X atom and the bare SiNW (i.e. no surface passivation), respectively. The isosurface of the charge density difference is plotted using the XCrySDen software [28].

3 Results and discussion

The cross-sections of the optimized hydrogen, fluorine, and hydroxyl passivated ⟨110⟩ SiNWs considered in this work are shown in Fig. 1b. We focus on studying three electronic properties: the Fermi level (FL, E_f), vacuum potential (VP, φ) and work function (WF, Φ) because $\Phi = \varphi - E_f$. Our investigations are divided into 4 parts: First, we evaluate the methodology. Second, we examine the effect of vacuum thickness on the electronic properties of hydrogen passivated SiNW (H-SiNW). Then, we study the diameter-electronic properties dependence using the H-SiNWs with diameters of 1.1, 1.5 and 2.3 nm. More importantly, in addition to the H-SiNW, we investigate the surface effects for the fluorine passivated SiNW (F-SiNW) and hydroxyl passivated SiNW (OH-SiNW) with different percentage of coverage.

3.1 Results for bulk silicon

Our method evaluation is done by comparing the calculated bulk silicon structure with experimental structure data (see Table 1). It is found that the calculated Si–Si bond length and the lattice constant deviated by less than 1% (~0.03 Å) from experimental data [29]. We thus adopt this method for the calculations of the SiNWs.

3.2 Vacuum thickness dependent work function

We adopt the H-SiNW with a diameter of 1.1 nm ($Si_{48}H_{32}$) for the calculation. To determine the work function, we need to calculate the average vacuum potential of the supercell. We plot the average vacuum potential as a function of cell length for the H-SiNW in a cell of different volume as shown in Fig. 2a. It is shown that the vacuum potential is around 4 eV in a small supercell (12 × 12 × c Å^3)

Fig. 1 **a** An example used to illustrate the unit cell used for the optimization of SiNWs. **b** Cross-sections of the H-SiNWs, F-SiNWs and OH-SiNWs with ⟨110⟩ growth orientation. *Axes* indicate the orientations of the nanowire. The surface orientations are labeled in $Si_{84}H_{40}$ as the example

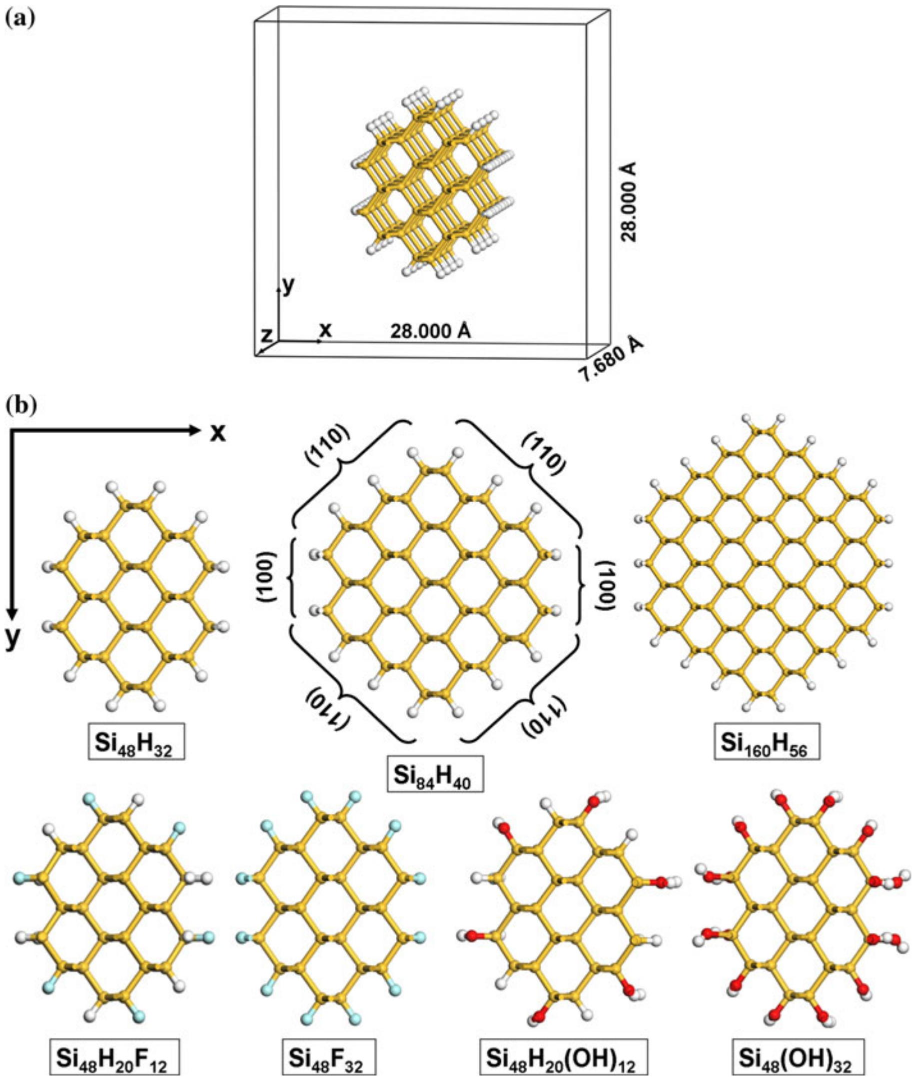


Table 1 Comparisons of Si–Si bond and lattice constant of bulk silicon

Stoichiometry	Si–Si bond (Å)	Lattice constant (Å)
Bulk Si (Si_8)	2.37	5.47
Expt.[a]	2.35	5.43

[a] Ref. [29]

while it approaches 0 eV in a large cell (82 × 82 × c Å^3). Data are presented in Table S1 in Supplementary Material.

To get the general trend, we plot the energies of WF, VP and FL as functions of vacuum thickness in Fig. 2b. It is shown that the average vacuum potential and the Fermi level decrease with increasing vacuum thickness, which tend to saturate at around 0 and –4.6 eV when the vacuum thickness is 25 Å, respectively. However, the work function of the H-SiNW remains almost constant at 4.61 eV which is independent of the vacuum size beyond 25 Å. This indicates that the work function of SiNW can be determined using a small supercell but a very large supercell has to be used if the work function is approximated as the negative value of the Fermi level, i.e. to keep the vacuum potential to almost 0 eV. Hence, we adopt a vacuum thickness of 25 Å for the rest of the calculations.

3.3 Diameter dependent work function

A plot of the energies of WF, VP and FL as functions of diameter for H-SiNW is shown in Fig. 3. Here we consider the H-SiNWs with 1.1, 1.5 and 2.3 nm diameters. It is shown that the average vacuum potential increases slightly with increasing diameter of the SiNWs. They are ~0, ~0.25, and ~0.5 eV for the H-SiNWs with 1.1, 1.5 and 2.3 nm diameters, respectively. It implies that a thicker vacuum is needed for the SiNW with a large diameter in order to keep the vacuum potential to almost 0 eV in the supercell. Data are presented in Table S2 in Supplementary Material.

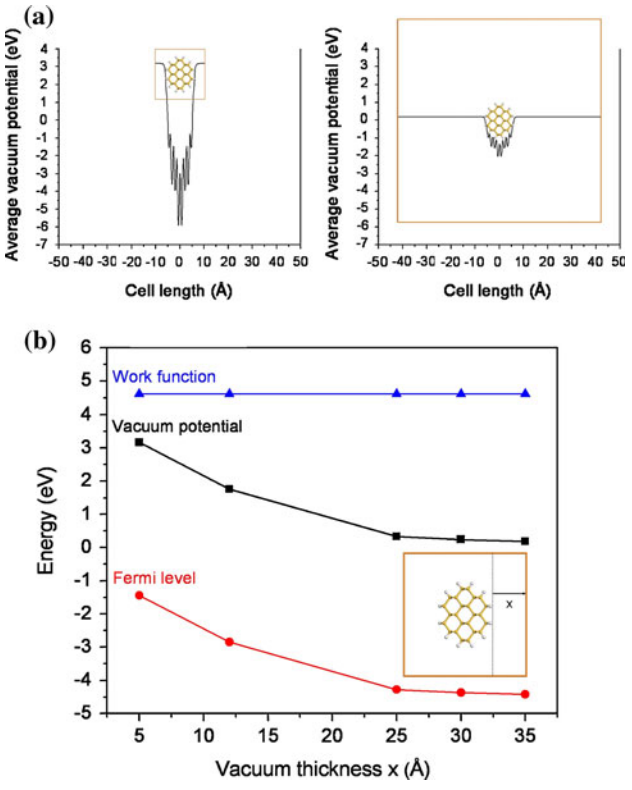


Fig. 2 **a** Plots of average vacuum potential as a function of cell length for the H-SiNW with a diameter of 1.1 nm. **b** A plot of work function, vacuum potential and the Fermi level as functions of vacuum thickness for the H-SiNW

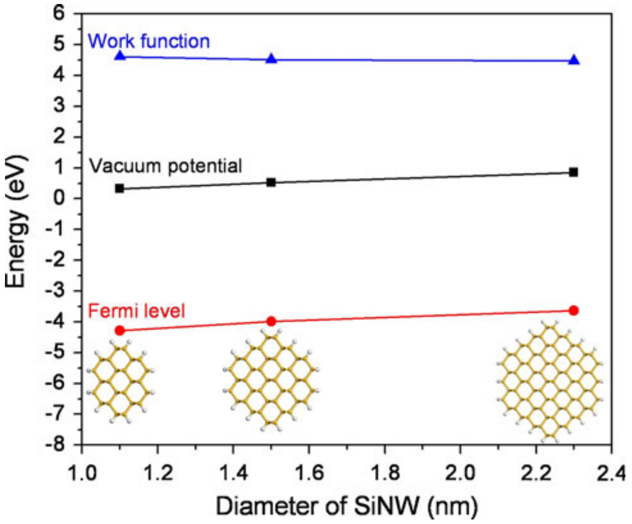


Fig. 3 A plot of work function, vacuum potential and the Fermi level as functions of diameter for the H-SiNWs

Table 2 The formation energies (E_F) per Si atom of the nanowires

Stoichiometry	$\frac{1}{n_{Si}} E_F$ (eV)
100% F ($Si_{48}F_{32}$)	–2.17
50% F ($Si_{48}H_{20}F_{12}$)	–0.83
100% H ($Si_{48}H_{32}$)	0.08
50% OH ($Si_{48}H_{32}O_{12}$)	–1.91
100% OH ($Si_{48}H_{32}O_{32}$)	–2.25

More importantly, it shows that the work function increases as the diameter decreases. The work functions for the ⟨110⟩ H-SiNWs with diameters of 1.1, 1.5 and 2.3 nm are 4.61, 4.51 and 4.48 eV, respectively. Our calculated results agree well with the theoretical work reported by Leu et al. [12] in which the work function of the ⟨110⟩ SiNW increases gradually with decreasing diameter. In their work, they compared the WF of both the ⟨110⟩ and ⟨111⟩ H-SiNWs with different diameters. They revealed that the WF of the ⟨110⟩ SiNW increases with decreasing diameter but the WF of the ⟨111⟩ SiNW is mostly size independent. Further investigation showed that the surface dipole effect, which is calculated in term of $V_{\text{ref}} - \varphi$ where V_{ref} is the average electrostatic potential at the core of the Si atoms in the SiNW and φ is the vacuum level, is the reason for the increased WF for the ⟨110⟩ SiNW with decreasing diameter [12].

Since the decay of work function with increasing size is roughly exponential, it is expected that the extrapolated work function for the H-SiNW with a very large diameter converges at about 4.4 eV. The extrapolated value agrees with the experimental value of 4.6 eV obtained from vertically aligned SiNWs after hydrogen plasma etching [30].

3.4 Surface composition dependent work function

Before comparing the work function of the surface passivated SiNWs, we compare their formation energies. With reference to the work published by Aradi et al. [31], the formation energy (E_F) is calculated by the formula: $E_F = E_{NW} - \sum_{i=Si,O,H,F} n_i\mu_i$ where E_{NW} is the total energy for a given nanowire and n_i and μ_i are the number and chemical potential of the elements. The theoretical chemical potential for Si is taken from the bulk silicon while the chemical potentials for O, H, and F are taken from their molecular states. As mentioned in Ref. [31], this approach neglects the effect of zero-point vibration and the pressure and temperature dependence of the chemical potentials, but it should give a reasonable comparison of stability. The results are presented in Table 2. The positive energy of H-SiNW indicates that it is metastable construct [32]. This result also agrees with that in Ref. [31]. Compared to H-SiNW, the F-SiNWs and OH-SiNWs are more stable. The stability trend is OH-SiNW > F-SiNW > H-SiNW, and the 100% coverage of the passivating atoms are more stable than the 50% one. It shows that the dangling bonds are passivated better in term of energy by the OH and F atoms than H atom, which may attribute to the intrinsic electronegative nature of O and F atoms.

A plot of the energies of WF, VP and FL as functions of surface composition for the H-SiNW, F-SiNW and OH-SiNW is shown in Fig. 4. Taking the H-SiNW as the reference, the work functions of the two F-SiNWs (50 and 100% coverage) are larger while the two OH-SiNWs (50 and 100% coverage) are smaller. The increase in work function for the F-SiNWs can be ascribed to the high electronegativity of F atom [33]. F atoms withdraw electrons from the surface of the SiNW, leading to an increase of charge density around the F atoms. The negative end of the induced dipole thus point towards the vacuum. As a result, the surface dipole is enhanced, leading to an increased work function for the F-SiNW (vs. H-SiNW, 4.61 eV). In addition, since such dipole enhancement is localized, the SiNW with 100% F coverage has a larger work function (6.73 eV) than the SiNW with 50% F coverage (5.31 eV). Data are presented in Table S3 in Supplementary Material.

For the SiNWs with 50 and 100% OH coverage, they both have smaller work functions than that of the H-SiNW, although an O atom is more electronegative than a H atom. To understand this phenomenon, we compare the surface structures of the SiNWs with 100% coverage of H, F, and OH (see Fig. 5). Here, we focus on the Si–Si bonds along the axial direction, i.e. the zigzag Si–Si bonds. For the H-SiNW, the surface Si–Si bonds (2.385–2.378 Å) are slightly shorter than the core Si–Si bonds (2.393 Å), indicating that H passivation would cause surface contraction. For the F-SiNW, the overall Si–Si bonds are elongated as compared to that of the H-SiNW. Within the F-SiNW itself, the surface Si–Si bonds are partly elongated (2.497 Å) or contracted (2.484 Å) as compared with the core Si–Si bonds (2.491 Å), depending on the local passivating environment. In general, the H-SiNW and F-SiNW have homogenous zigzag Si–Si bonds at both the surface and the core.

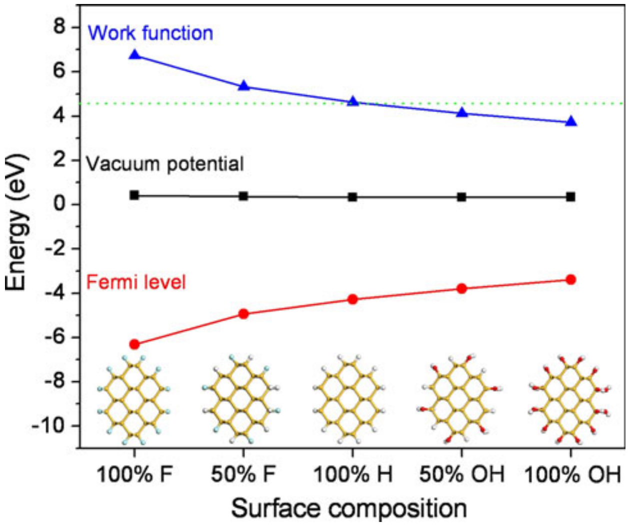
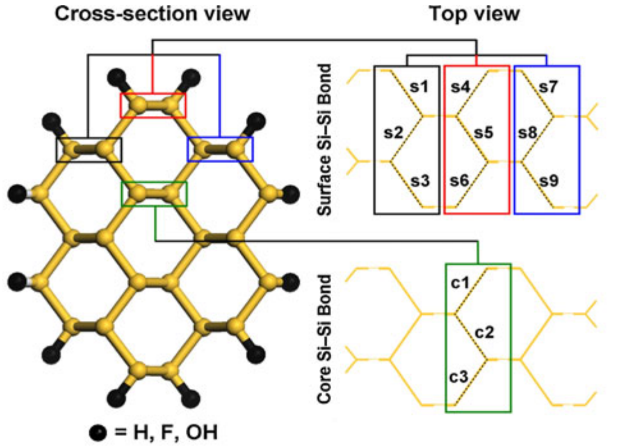


Fig. 4 A plot of work function, vacuum potential and the Fermi level as functions of surface composition for the H-SiNW, F-SiNWs and OH-SiNWs. The *green dotted line* indicates the work function of the H-SiNW for comparisons



	Surface Si–Si bond (Å)			Core Si–Si bond (Å)
F-SiNW	s1 = 2.497	s4 = 2.484	s7 = 2.497	c1 = 2.491
	s2 = 2.497	s5 = 2.484	s8 = 2.497	c2 = 2.491
	s3 = 2.497	s6 = 2.484	s9 = 2.497	c3 = 2.491
H-SiNW	s1 = 2.385	s4 = 2.378	s7 = 2.385	c1 = 2.393
	s2 = 2.385	s5 = 2.378	s8 = 2.385	c2 = 2.393
	s3 = 2.385	s6 = 2.378	s9 = 2.385	c3 = 2.393
OH-SiNW	s1 = 2.386	s4 = 2.373	s7 = 2.386	c1 = 2.387
	s2 = 2.344	s5 = 2.428	s8 = 2.344	c2 = 2.434
	s3 = 2.386	s6 = 2.373	s9 = 2.386	c3 = 2.387

Fig. 5 Comparison of surface and core Si–Si bond lengths for the SiNWs with 100% coverage of F, H and OH. *Yellow* and *black balls* indicate the Si and passivating (F, H and OH) atoms. SiNWs in top view are shown in *line* drawing for clarity to show the Si–Si bond lengths

However, it is different for the OH-SiNW. OH passivation would induce conjugate-liked zigzag Si–Si bonds on the surface and core of the SiNW as shown in Fig. 5. The core Si–Si bonds alternate between 2.387 and 2.434 Å while the surface Si–Si bonds alternate between 2.386 and 2.344 or 2.373 and 2.428 Å, also depending on the local passivating environment. We attribute this observation to the fact that the OH group has the electron resonance effect towards the surface of the SiNW, i.e. electron is donated back to the surface of the SiNW, resulting in conjugate-liked zigzag Si–Si bonds. Such resonance effect from the OH group could override the electronegativity effect of O atom, resulting in reduced dipole on the surface of the SiNW and a reduction of work function (vs. H-SiNW, 4.61 eV). Similar to the case of F-SiNW, such dipole reduction is localized: the OH-SiNW with a 100% OH coverage has a smaller work function (3.72 eV) than the OH-SiNW with a 50% OH coverage (4.11 eV).

We have also calculated the charge density difference (CDD) between the passivating atoms and the SiNW. The CDD indicates the net charge as a result of the two interacting systems. The isosurface plots of the CDD for the SiNWs with 100% H, F and OH coverage are shown in Fig. 6. From the CDD plots, it is shown that there is no net charge in the SiNW core, i.e. the charge transfer only occurs between the passivating atoms and the outermost surface Si atoms.

For the H-SiNW, the net charge is mostly located around the H atoms, indicating that the H atoms draw electrons from the SiNW surface. This is because H atom is more electronegative than Si atom. A similar phenomenon is observed for the F-SiNW because F atom is even more electronegative than H atom. In contrast, for the OH-SiNW, the net charge is located at both the OH groups and near the SiNW surface. It can be observed that some net charges are accumulated between the Si–Si bonds near the SiNW surface (indicated by dotted squares in Fig. 6). This is because the (100) surface is di-substituted by the OH groups, i.e. two OH groups bond to a Si atom. The electron resonance effect is much stronger than that of the mono-substituted (110) surface (see Fig. 1b for the surface orientation).

To further examine the surface orientation effects, we examine another two OH-SiNWs in which the OH groups on the (100) and (110) surfaces are replaced by H atoms, respectively, as shown in Fig. 7a. In the case when the (100) surfaces are replaced by H atoms, the calculated work function of this OH-SiNW is 4.29 eV (vs. H-SiNW, 4.61 eV), showing that there is moderate reduction of work function. Such reduction of work function is due to the resonance effect of OH groups on the (110) surfaces that donate electron back to the surface. In comparison, when the (110) surfaces are replaced by H atoms, the work function of this OH-SiNW is lowered to 3.82 eV (vs. H-SiNW, 4.61 eV), showing a much stronger reduction of work function. As such, surface modification on the di-substituted (100) surfaces should result in a stronger effect to modulate the work function for SiNWs. The CDD plots for these two OH-SiNWs are shown in Fig. 7b. The results indicate that the work function of the SiNW is very sensitive to the nature of chemical bonding as well as the surface orientations.

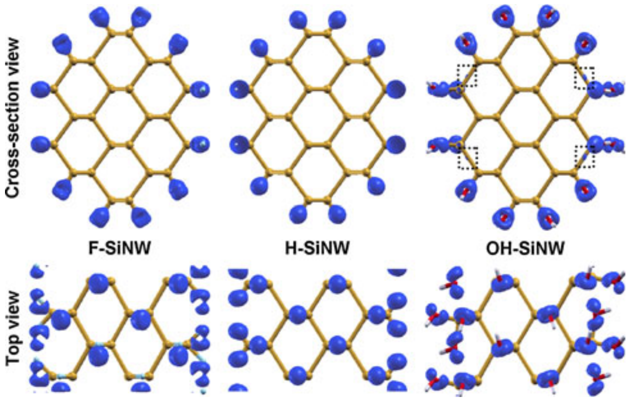


Fig. 6 The isosurface plots (*blue*) of charge density difference for the SiNWs with 100% coverage of F (*left*), H (*middle*) and OH (*right*). The *dotted squares* within the OH-SiNW indicate the charge density located at Si–Si bonds. The isovalue is set at 0.09

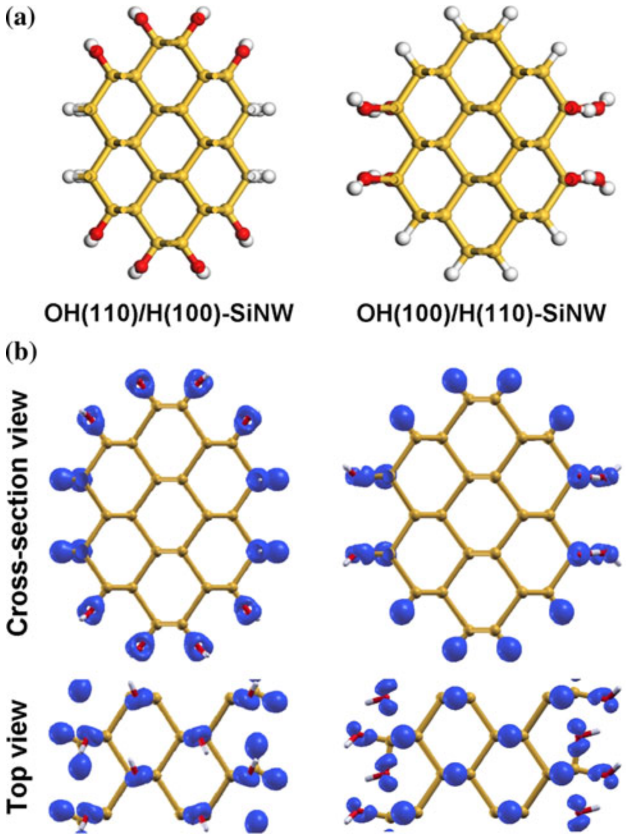


Fig. 7 **a** The cross-sections of the OH-SiNWs with the (100) surfaces (*left*) and (110) surfaces (*right*) replaced by H atoms. **b** The isosurface plots (*blue*) of charge density difference for the SiNWs. The isovalue is set at 0.09

Overall, the increase of electron density on the surface of the SiNW would result in a reduction of work function. In addition, we propose that such electron enhancement near the surface of the SiNW by the OH groups is the reason to cause the conjugate-liked surface and core Si–Si bonds in the OH-SiNW, i.e. a resonance-liked effect due to the OH passivation.

4 Conclusion

We have used DFT calculations to evaluate the electronic structures and work functions of hydrogen, fluorine, and hydroxyl passivated SiNWs. We show that the calculation of work function does not depend on the vacuum thickness of the supercell for SiNWs, but the Fermi level requires a vacuum thickness of at least 25 Å to converge for the SiNW with a diameter of ~ 1 nm. Also, our calculated work function of SiNW agrees with experimental data. More importantly, we reveal that the work function of SiNW depends strongly on the electron withdrawing effect and resonance effect of the passivating atoms. A trend of work functions: F-SiNW > H-SiNW > OH-SiNW, is obtained. We show that the F-SiNW and OH-SiNW have an increased and reduced work function as compared to that of the H-SiNW, respectively. The former is due to the highly electronegative F atom that weakens the surface dipole on the SiNW surface. The latter is attributed to the resonance effect in which electron is donated back to the surface, resulting a strengthened surface dipole and conjugate-liked surface and core Si–Si bonds within the SiNW. This is supported by our charge density difference analysis. In addition, we show that the formation energies for the surface passivated SiNWs are in the stability order of OH-SiNW > F-SiNW > H-SiNW. Work function remains one of the important parameters to be considered for selecting materials in device design. The present results suggest that surface modifications can be used to modify the work function of SiNW for customize purpose.

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