

EP06

Antiferromagnetic Coupling of the Dangling Bonds on Si(001) Surfaces

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Dangling bonds (DBs) can be produced by the desorption of hydrogen (halogen) atoms from the hydrogen(halogen)-terminated Si(001)-2×1 surface [1] or by the adsorption of C₆₀ molecules on Si(001)-2×1 surface [2]. There is the interdimer DB configuration where two DBs are on one side of two adjacent Si dimers (see Fig. 1). The hitherto accepted structural model for the interdimer configuration of DBs is based on the nonmagnetic (NM) state which contains the up and down displaced DBs because of the presence of two alternatively buckled dimers along the dimer row (see NM in Fig. 1). However, using spin-polarized density functional theory calculations, we predict that two adjacent DBs are antiferromagnetically coupled with each other on the hydrogen (halogen)-terminated Si(001)-2 × 1 surface [3] and on the C₆₀ adsorbed Si(001)-2 × 1 surface [4]. Our electronic-structure analyses for such an antiferromagnetic (AFM) state which consists of the symmetric dimers (see AFM in Fig. 1) provide good explanations for a scanning-tunneling-microscopy image of the interdimer configuration on hydrogen-terminated Si(001) as well as for photoelectron spectroscopy data of the C₆₀ adsorbed Si(001) surface.

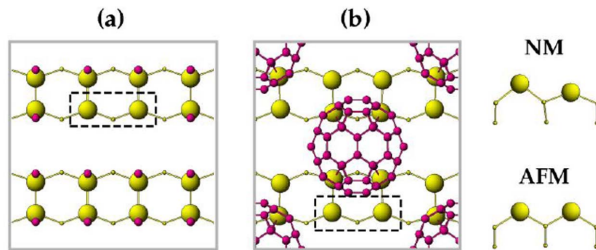


Fig. 1. Top views of the interdimer configuration of DBs on (a) hydrogen (halogen)-terminated Si(001) and (b) C₆₀-covered Si(001). The largest balls represent Si dimers, while the medium ones represent hydrogen (halogen) atoms in (a) and carbon atoms in (b). Two Si DBs within the interdimer configuration are included in the shaded boxes. On the right side of (b), the side views of the NM and AFM states for the interdimer configuration are displayed.

REFERENCES

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EP07

Calculation of Electronic Structures and Magnetic Properties of α -quartz SiO₂ with and without Transition Metal Elements

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Electronic structures and magnetic properties of pure α -quartz SiO₂ and doped α -quartz Si_{1-x}M_xO₂, which M represents the transition metals V, Cr and Mn, are calculated using Hartree Fock (HF) and Density Functional Theory (DFT) methods. The results show that the energy gaps of Si₁₈O₂₆H₃₂ calculated by HF and DFT methods are 15.766 eV and 7.560 eV respectively and those of doped α -quartz SiO₂ calculated by both methods are found to reduce and the most narrow one is found in Si₁₇CrO₂₆H₃₂ (see Table 1). The total dipole moments of doped α -quartz SiO₂ are higher than that of pure α -quartz SiO₂ except the doping by V. In addition, the highest value of total dipole moment as listed in Table 2 is found in Si₁₇MnO₂₆H₃₂.

Table 1. The Energy gaps of pure and doped α -quartz SiO₂ calculated by HF and DFT methods.

Structure	Energy gap (eV), E _g	
	HF method	DFT method
Si ₁₈ O ₂₆ H ₃₂	15.766	7.560
Si ₁₇ VO ₂₆ H ₃₂	4.359	1.760
Si ₁₇ CrO ₂₆ H ₃₂	10.074	1.263
Si ₁₇ MnO ₂₆ HS	10.062	3.091

Table 2. The values of total dipole moments of each SiO₂ structure calculated by HF and DFT methods.

Structure	Total dipole moments (Debye)	
	HF method	DFT method
Si ₁₈ O ₂₆ H ₃₂	4.0479	3.6332
Si ₁₇ VO ₂₆ H ₃₂	3.5726	2.7683
Si ₁₇ CrO ₂₆ H ₃₂	4.7830	4.3398
Si ₁₇ MnO ₂₆ H ₃₂	5.1349	4.5009