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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 C_{60} 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 C_{60} 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 C_{60} adsorbed Si(001) surface.

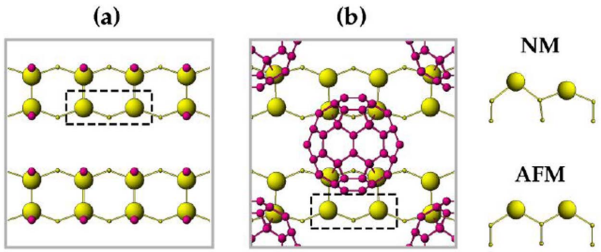

Fig. 1. Top views of the interdimer configuration of DBs on (a) hydrogen (halogen)-terminated Si(001) and (b) C60-covered Si(001). The largest balls represent Si dimers, while the medium ones represent hydrogen (halogen) atoms in (a) and carbon atoms in (b). Two Si DBs within the interdimer configuration 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.

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Calculation of Electronic Structures and Magnetic Properties of α-quartz SiO_2 with and without Transition Metal Elements

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Electronic structures and magnetic properties of pure α-quartz SiO_2 and doped α-quartz $Si_{1-x}M_x O_2$, 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 $Si_{18}O_{26}H_{32}$ calculated by HF and DFT methods are 15.766 eV and 7.560 eV respectively and those of doped α-quartz SiO_2 calculated by both methods are found to reduce and the most narrow one is found in $Si_{17}CrO_{26}H_{32}$ (see Table 1). The total dipole moments of doped α-quartz SiO_2 are higher than that of pure α-quartz SiO_2 except the doping by V. In addition, the highest value of total dipole moment as listed in Table 2 is found in $Si_{17}MnO_{26}H_{32}$.

Table 1. The Energy gaps of pure and doped α-quartz SiO_2 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 SiO_2 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