Electronic structure and optical properties of Si(111)/SiO_2 plane interface.

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Interfaces between two materials, among them Si/SiO_2, play an important role in the semiconductor industry in particular for the complementary metal-oxide-semiconductor (CMOS) technology and for fabrication of light-emitting Si-based nanostructured materials. Silicon - silicon dioxide plane interfaces computationally designed in Ref. [1] belong to nanostructured materials with one-dimensional (1D) nanoscale.

In the present work we study the electronic structure of silicon dioxide interface with the (111) silicon surface; it is equivalent to the {$Si_{66}O_{40}$-111} interface presented in Ref. [1], except that the Si-atoms in new model are placed inside the cell. The interface is designed for the purposes of atomic modeling of surface photovoltage, similar as it was done for the Si(111):H surface [2].

In the present study the calculations were carried out using density functional theory (DFT) in the generalized gradient approximation (GGA) with plane waves (PW) and pseudo-potentials (PP) as implemented in `VASP` [3]. Structural relaxation was performed without any symmetry constraints except that the lattice was kept orthorhombic during optimization. Kinetic energy cutoff used in PW basis set is 495 eV. The binding energy (in eV per SiO_x unit, x=0.606 for our model) is found to be 10.25 eV which is very close to the value of 10.52 eV of the *stress* energy calculated in Ref. [1]. The lattice cell parameters are 7.529x6.601x36.081 angstrom. The band structure was calculated using 11x11x1 Monkhorst – Pack uniform ***k***-point grid. The band structure in $\boldsymbol{k}_z$ direction is dispersion less (the dispersion less of band structure in that direction was found in Refs. [4,5]). The band gap in interface is almost direct, the energy gap in Γ-point is 1.55 eV. Finally, optical properties, as given by the imaginary part of the dielectric function are calculated using numerical atomic orbital (NAO) basis set as implemented in `SIESTA` [6].

References

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