Electronic State and Chemical Bonding of TiO_2 (110) Surface, Calculated Using Cluster Method

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The surface states and chemical bonding of atoms on the TiO_2 (110) surface were calculated using discrete variational X_α (DV-X_α) method, which is a sort of the first principles molecular orbital method and uses Hartre-Fock-Slater approximation. Various models based on the (110) (1x1) structure were constructed to investigate the variation of surface states and chemical bonding between surface atoms with the existence of a surface vacancy and adsorbed oxygen. The calculated results involve the energy level, the density of state (DOS), the overlap population diagram, the net ionic charge, and wave functions. Discussions are focused on the surface levels introduced by defects and the bonding state between Ti and oxygen. As results, the formation of surface levels was related to the surface charge and the charge transfer of electrons from the under-surface oxygen to the surface oxygen. However, the overlap population between Ti and O was not affected by the surface charge.

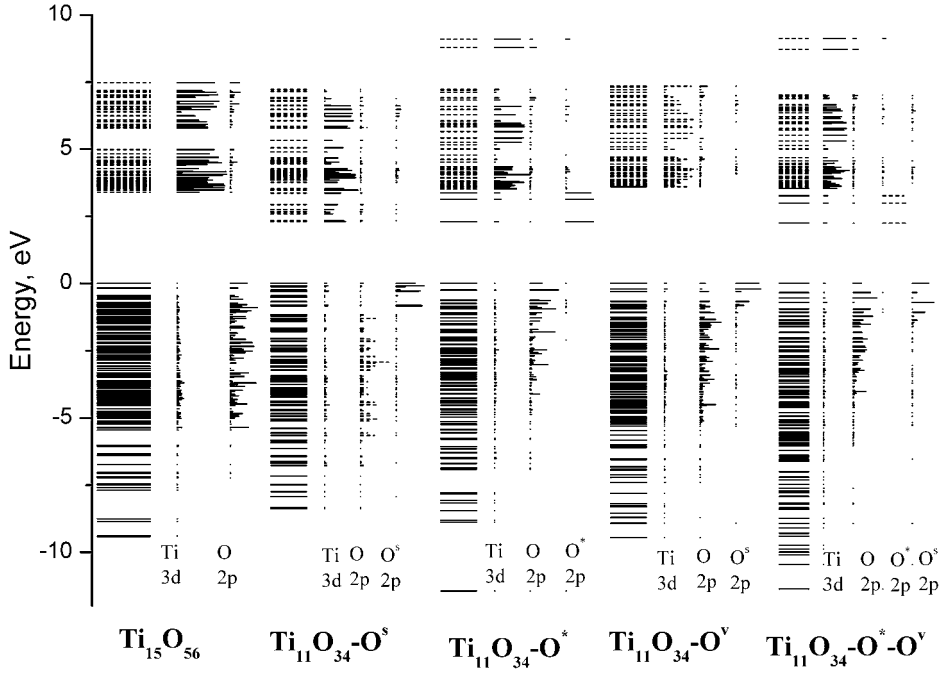

Fig.1. The energy levels calculated using the various cluster models of TiO_2 (110) (1x1) surface. The electron filled surface levels under the conduction band were shown in the models with a surface vacancy and oxygen adsorption. The solid line indicates the electron filled level and the dotted line indicates the electron unfilled level. O^s, O^*, and O^v are the surface oxygen of (110) (1x1) structure, the oxygen adsorbed on the five folded Ti ion, and the oxygen vacancy related to (1x1) oxygen array, respectively.

References

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