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Study on TiO_2 Photocatalysis for Organics by Accelerated Quantum Chemical Molecular Dynamics Method

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【Introduction】

Photocatalytic reactions are useful for the treatment of air polluted with organic compounds. Hitherto, many researchers have investigated the photooxidation of organic pollutants and have reported that a variety of compounds, such as hydrocarbon, alcohols, chlorohydrocarbons and amines are decomposed on the UV-irradiated TiO_2 catalyst under ambient conditions. In this study, the photooxidation of CH_3Cl was carried out at room temperature. Moreover the results including a fully optimized ground-state structure obtained as well as the densities of states (DOS) are also presented.

【Method】

The accelerated quantum chemical molecular dynamics calculations were carried out using 'Colors' program, which is based on the tight-binding approximation. The Amsterdam density functional (ADF) program based on the density functional theory is also employed to determine the parameters for 'Colors'.

【Results and discussion】

We performed the quantum chemical calculations of the band structure of TiO_2 by 'Colors' program. The fully optimized structure was obtained by minimizing the total energy and atomic forces by 'Colors' program. We also acquired the Densities of States (DOS) of TiO_2 structure. Fig. 1. shows the DOS of TiO_2. From DOS, valence band composed by O 2p orbitals and conduction band composed by Ti 3d orbitals can be found easily at A point and B point of Fig. 1 respectively. Moreover the band gap energy of 3.15 eV, which is agreement with the experiment well, was attained. We also investigated the photodecomposition process of hydrocarbons. Fig. 2 shows the model of CH_3Cl-TiO_2 system. Our results show that these compounds can be decomposed on the TiO_2 catalyst.

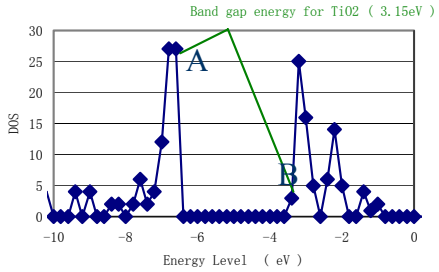

Fig.1. The DOS of TiO_2 structure.

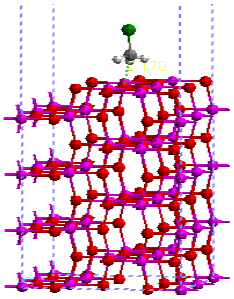

Fig.2. Model of CH_3Cl-TiO_2 system

References

1. A.L. Linsebigler et al., Phys. Rev. B, 95, 735-758 (1995).