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研究快报

二氧化钛(TiO_2)表面上水分解反应的理论研究

魏志钢[1,2], 李前树[2], 张红星[1], Lewis James P.[3]

1. 吉林大学理论化学研究所, 理论化学计算国家重点实验室, 长春 130023;
2. 北京理工大学化工与材料学院, 北京 100081;
3. 伯明翰姆·扬大学物理天文学系, 犹他 84602

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摘要 模拟了较大的反应体系, 希望能与实验进行比较, 更好地解释实验结果, 理解反应过程.

关键词 二氧化钛-金红石(TiO_2)表面 水分解 火球程序

分类号 0641

Theoretical Study of Water Decomposition on TiO_2 Surface

WEI Zhi-Gang[1,2], LI Qian-Shu[2], ZHANG Hong-Xing[1], Lewis James P.[3]

1. School of Chemical Engineering and Materials Science, Beijing Institute of Technology, Beijing 100081, China;
2. State Key Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin University, Changchun 130023, China;
3. Department of Physics and Astronomy, Brigham Young University, Provo, UT 84602, USA

Abstract Density functional theory and pseudopotential method were employed to investigate one water molecule decomposition on perfect TiO_2 rutile(110) surface. First we build up a surface, which is large enough to simulate this reaction as under the real condition. Then we put a water molecule on the top of one five-fold-coordinate Ti atom on the surface as the reactant; we put two OH radicals at the corresponding position of the surface as the product. At last we simulate the reaction from the reactant to the product to get the reaction free energy, which is about 15.562 kJ/mol. This free energy can fit well with the experimental results.

Key words TiO_2 Rutile surface Water decomposition Fireball program

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通讯作者 张红星 hxzhang@mail.jlu.edu.cn