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论文

二氧化钛(TiO_2)表面能的理论研究

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摘要:

用密度泛函理论和虚拟原子轨道方法对二氧化钛-金红石(TiO_2)(110)表面的表面能进行了理论计算. 结果表明, 二氧化钛的表面能与表面缺陷的百分率相关. 完整的表面具有最低的表面能, 表面能随着表面缺陷百分率的增大而升高, 这与自然环境下二氧化钛-金红石(TiO_2)具有规整的(110)表面一致. 在光催化实验中利用二氧化钛表面的缺陷作催化剂需要考虑到表面的稳定性. 另一方面, 在完整的表面五配位Ti^{4+}上填加氧原子与表面作用时, 表面能起初变化很小, 直到50%的五配位Ti^{4+}被填充后表面能才开始升高.

关键词: 二氧化钛-金红石(TiO_2)(110)表面 表面能 缺陷表面 火球程序

Theoretical Study on the Surface Energy of TiO_2 Rutile(110)

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Abstract:

The density functional theory and pseudopotential method were employed to investigate the TiO_2 rutile (110) surface energy corresponding to the defect concentration. It is shown that the surface energy is dependent on the defect percentage, *i.e.*, the zero defect surface possesses the lowest surface energy and the 100.0% defect surface possesses the highest surface energy. On the other hand, when we added O atoms to the fivefold-coordinate Ti^{4+} sites of the perfect surface with a defect below 50%, there is little change of the surface energy, although the perfect surface still has the lowest surface energy. When we added more O atoms to these sites, the surface energy becomes higher.

Keywords: TiO_2 Rutile(110) surface Surface energy Defect surface Fireball program

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参考文献：

1. Diebold U.. Surf. Sci.[J], 2003, 48: 53—229
2. Epling W. S., Peden C. H. F., Henderson M. A., *et al*.. Surf. Sci.[J], 1998, 412: 333—343
3. Henderson M. A., Epling W. S., Perkins C. L., *et al*.. J. Phys. Chem. B[J], 1999, 103: 5328—5337
4. Charlton G., Howes P. B., Nicklin C. L., *et al*.. Phys. Rev. Lett.[J], 1997, 78: 495—498
5. Ramamoorthy M., Vanderbilt D., King-Smith R. D.. Phys. Rev. B[J], 1994, 49: 16721—16727
6. Bates S. P., Kresse G., Gillan M. J.. Surf. Sci.[J], 1997, 385: 386—394
7. Lewis J. P., Glaesemann K. R., Voth G. A., *et al*.. Phys. Rev. B[J], 2001, 64: 195103—195112
8. Wang H., Lewis J. P.. J. Phys.: Condens Matter[J], 2005, 17: 209—213
9. Burdett J. K., Hughbanks T., Miller G. J., *et al*.. J. Am. Chem. Soc.[J], 1987, 109: 3639—3648
10. Wang S. G., Wen X. D., Cao D. B., *et al*.. Surf. Sci.[J], 2005, 577: 69—76

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