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TiB2(0001)表面性质的密度泛函理论

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摘 要：用第一性原理方法分析两种TiB_2(0001)表面的几何和电子结构。结果表明：两种TiB_2(0001)表面都不发生重构，但表面几层原子都出现明显的弛豫现象，其中以终止于硼原子的表面弛豫尤为明显，而终止于钛原子的表面相对较稳定，弛豫较轻；进一步对两种不同表面的表面能分析表明，终止于钛原子的表面在更宽的范围内具有较低的表面能；这些结果说明，终止于钛原子的表面较稳定。

关键字： TiB2(0001)表面；密度泛函理论；表面弛豫；表面能

Density functional theory on characteristics of TiB2 (0001) surface

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Abstract: The geometry and electronic structure of two different TiB2 (0001) surface were investigated by the method of density functional theory. The results indicate that there will be no reconstruction phenomenon for both different TiB2 (0001) surfaces, while there will be obvious relaxation, especial for the B-terminated surface, in top-three layers. The surface energies of the two kinds of surfaces are also analyzed. The results show that the surface energy of Ti-terminated is lower in much wider range compared with that of B-terminated surface. So it can be believed that Ti-terminated surface maybe the stable TiB2 (0001) surface.

Key words: TiB2 (0001) surface; density functional theory; surface relaxation; surface energy

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