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铝晶体自由表面的稳定性计算

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摘 要：采用第一原理赝势平面波方法，计算铝晶体学自由表面(100)、(110)和(111)的能量、几何与电子结构。根据表面能计算预测铝自由表面结构的稳定性。结果表明：铝自由表面结构稳定性由强到弱的顺序为(111)、(100)、(110)；表面原子驰豫不仅引起表面几何结构的变化，而且使表面层的电子结构与键合特性发生改变；(100)、(110)和(111)表层驰豫分别为3.337%、−6.147%和−2.364%；表面电荷密度不同引起表面能差异，表面原子层和次表面原子层的电荷面密度在s和p轨道上重新分布；表面原子层电荷密度越大，表面能越低。

关键字：Al晶体；第一原理；表面驰豫；表面能

Calculation of stability of free surfaces in aluminum crystal

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Abstract: The surface energy, atomic geometry and electronic structures of Al(100), (110) and (111) free surfaces were calculated using the method of supercell and the first-principles pseudopotential plane waves within generalized gradient approximation. According to the calculated surface energy, the structural stability of Al free surfaces from strong to weak is predicted in the order as (111), (100) and (110). The relaxation of the surface atom layers not only causes the change of geometrical structures of the surface models, but also leads to the variation of their electronic structures and bonding characters. For the (100), (110) and (111) free surfaces, the calculated surfaces relaxation are 3.337%, −6.147% and −2.364%, respectively. The surface energy is related to the surface electron density distribution, the electron density of orbital s and p of the first two surface atom layers redistributes. The higher the surface electron density is, the lower the surface energy is.

Key words: aluminum crystal; first principle; surface relaxation; surface energy

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