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不同晶型氢氧化铝的反应活性与微观键力分析

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摘 要： 根据实验晶格参数构建3种不同类型氢氧化铝——三水铝石、拜耳石及诺耳石的晶体结构模型，基于密度泛函理论(DFT)的广义梯度近似(GGA)和局域密度近似(LDA)方法，用CASTEP程序分别对各研究体系进行几何优化，计算各体系的总能量、电子结构、原子布居和键布居数。计算结果表明：在原子类型和数目相同的条件下，三水铝石总能量最低，即最稳定；GGA-PW91基组的能量效应最高，在相同计算精度下，计算结果更收敛；GGA-PW91及LDA-CA-PZ基组水平的能带结构和态密度的计算结果表明，3种氢氧化铝晶体能隙的最低值差别不明显，但三水铝石能隙的最高值比其他2种的低，从侧面反映了三水铝石的反应活性可能稍高；布居分析结果表明，三水铝石的H—O键和Al—O键的布居数最小，说明三水铝石较拜耳石和诺耳石H—O键和Al—O键的结合力最小，理论上三水铝石更有利于煅烧成氧化铝。

关键字： 氢氧化铝；密度泛函理论；电子结构；布居分析

Reactive ability and bond strength analysis on A l(OH)$_3$ crystals with three different crystallines

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Abstract: Crystal structure models of Al(OH)$_3$ crystals with three kinds of crystallines, which are gibbsite, bayerite and nordstradite, were built respectively according to the corresponding experimental crystal lattice. Geometry optimizations were implemented by CASTEP program module using general gradient approximation (GGA) and local density approximation (LDA) methods respectively based on density functional theory (DFT). The total energy, electronic structure, atomic and bond populations were also calculated. The calculation results of total energy indicate that gibbsite is more steady than the other two according to energy, and the effect of basis set of GGA-PW91 is the highest. Energy bond structure and density of states calculated at GGA-PW91 and LDA-CA-PZ levels show that the difference of energy gap ΔE ($E_{\mathrm{LUMO}}-E_{\mathrm{HOMO}}$) at the first group of BZ is not obvious, and that the highest value of ΔE of gibbisite is more lower than that of the other two Al

$(OH)_3$ crystals. Gibbisite may be more active than the other two crystals. The bond populations value of H—O and Al—O bonds of gibbisite is the smallest in three different $Al(OH)_3$ crystals. This is to say that the combination force of H—O and Al—O bonds of gibbisite is the smallest and gibbisite may be more easier to be calcined into alumina theoretically.

Key words: $Al(OH)_3$; DFT; electronic structure; population analysis