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ZHONGNAN DAXUE XUEBAO(ZIRAN KEXUE BAN)

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氢氧化铝有利生长基元$[Al_6(OH)_{18}(H_2O)_6]_n$微观叠合的DFT计算

吴争平，尹周澜，陈启元，李 洁

(中南大学 化学化工学院 化学工程与技术博士后流动站，湖南 长沙，410083)

摘 要：以氢氧化铝有利生长基元叠合模型为研究对象，用基于密度泛函理论(DFT)的DMol3程序计算各种典型基元$[Al_6(OH)_{18}(H_2O)_6]_n$($n$=3，4，5，6，7，8)叠合体系的总能量、结合能、基元团间相互作用能及轨道能量等，获得氢氧化铝有利生长基元分子叠合的键力特征等微观图像。研究结果表明，当叠合基元数n相同时，“正面正对叠合”模型的能量稳定性最高，结合力最强；整体上，“正面型”基元团能量的稳定性较高，结合力较强；叠合基元数n对不同叠合方式构建的少基元叠合模型的影响趋势是不同的，对于“侧棱”型叠合，n越大，体系的稳定性越低；对于“正面”型叠合，n越大，体系的稳定性越高；随叠合基元数n的增大，“正面”叠合少基元体系相互吸引的作用力增强，而“侧棱”叠合体系的基元间相互作用能$E_{(VDW)}$相互排斥的作用力更强；“正面”型叠合是有利于形成较稳定的新相生成基元团的叠合方式，以“正面”叠合为主形成的基元团更有可能形成晶体生长过程中的原始晶胚。

关键字：氢氧化铝；有利生长基元；微观叠合；密度泛函理论

DFT calculation on microcosmic combination of favorable growth unit of gibbsite $[Al_6(OH)_{18}(H_2O)_6]_n$

WU Zheng-ping, YIN Zhou-lan, CHEN Qi-yuan, LI Jie

（Postdoctoralexchange Station of Chemical Engineering and Technology, School of Chemistry and Chemical Engineering, Central South University, Changsha 410083, China）

Abstract: The total energy, binding energy, interaction reaction energy and orbital energy of kinds of typical $[Al_6(OH)_{18}(H_2O)_6]_n$ (n=3, 4, 5, 6, 7, 8) units combination systems were calculated using DMol3 program based on density functional theory (DFT), the microcosmic characterization of the combination of the favorable growth unit of Gibbsite was obtained. The calculation results indicate that the stability and bonding strength of “face-face combination” model are the highest, and on the whole, the stability and bonding strength of “face type” combination models are higher than those of the “side type” models. The effect of the increase of combination value n on the systems’ stability is different between “side type” and “face type”. The stability of the “face type” combination modes is enhanced with the increase of the combination value n, and the “side type” modes is just reversed. When the number of “n” is increased, the attract force of the “face type” modes and the repulsion force of the “side type” are both stronger. It can be confirmed that the “face type” is the favorite combination modes which are

advantaged to the nucleation process, and the growth unit group with “face type” combination will be easier to form original crystal nuclear.

Key words:gibbsite; favorable growth unit; microcosmic combination; DFT