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外压对氢氧化铝晶体电子结构及谱学性质的影响

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摘 要： 用CASTEP程序计算不同外压下氢氧化铝的电子结构与谱学性质，分析外压对体系能带结构、态密度及光学性质的影响。计算方法选用基于密度泛函理论(DFT)的广义梯度近似(GGA)方法，用PBE函数进行交换相关系修正。能带结构计算结果表明，在较高外压下，如10.0和20.0 GPa，体系的能带结构较低外压下变化明显；体系各k-point点的能隙值随外压的增加均呈增大的趋势，由此也可预测外压应该对体系的光学性质有一定的影响。态密度计算结果表明，外压对最低能组态密度最高峰值影响最明显，其降低幅度分别达到15%和20%，价带所在能组态密度最高峰值随外应力增加的减弱幅度相对较小，而外压对最高能组态密度最高峰值几乎没有影响。光学计算结果表明，外压对氢氧化铝的光学性质有一定影响，其反射光谱和吸收光谱有明显变化，随外压的增大，体系的主要反射峰位和吸收峰位对应的能量呈变大的趋势，对应的反射系数和吸收系数均明显增大。外压对介电函数和导电系数的影响计算结果与对吸收光谱的影响是一致的。

关键字： 氢氧化铝；电子结构；谱学性质；外压

Electronic structure and optical properties of gibbsite crystal under different external stress

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Abstract: Electronic structure and optical properties of gibbsite under different external stresses were calculated using CASTEP program. The effects of external stress on bond structure, DOS and optical properties were analyzed. The calculation results indicate that the bond structure under higher external stress, such as 10.0 and 20.0 GPa, is more different than that under lower external stress, and the energy gap of every k-point of systems is increased with augment of external stress, that is to say, the external stress may have some effect on optical properties. The effect of external stress on DOS of the lowest energy group is very distinct, and the reduction is 15% and 20% respectively. The reduction of the energy group in which valence band locates, is less than the lowest energy group relatively, and there is hardly any effect of external stress on the highest energy group. The calculation results of optical properties indicate that with the increase of external stress, the energies of the main reflectivity and absorption peaks are increased, and the corresponding reflectivity and absorption

coefficient are increased distinctly. The effect of external stress on dielectric function and conductivity is consistent with the effect on absorption spectrum.

Key words: gibbsite; electronic structure; spectrum property; external stress

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