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研究论文

氨硼烷低温和室温结构的第一性原理计算

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摘要: 采用第一性原理平面波赝势方法研究了两种氨硼烷结构(Pmn21及P42cm)的晶格参数、电子结构以及动力学性质。结果表明, Pmn21结构的能量低于P42cm结构, 与实验观测结果相符, 即低温相为Pmn21结构而室温相为P42cm结构。Pmn21到P42cm相变所引起的结构变化主要体现为氨硼烷分子间双氢键键长显著增加, 而分子内部化学键键长变化不大。根据电子态密度分析了氨硼烷的成键状态。氨硼烷室温相的XRD图谱和FTIR图谱的理论预测结果与实验结果符合得较好。

关键词: 材料科学基础学科 氨硼烷 第一性原理 晶体结构 储氢材料

First--principles Study of Structure of Ammonia Borane

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Abstract: Two kinds of crystal structures (Pmn21 and P42cm) of (ammonia borane) are studied using first－principles plane wave pseudopotential method based on density functional theory in this paper. It was found that the Pmn21 structure is energetically more stable than the P42cm structure at 0 K. This agrees well with the experimental observation, that lower temperature phase is the Pmn21 structure whereas the room temperature phase is P42cm structure. The structure difference between Pmn21 and P42cm phases manifests itself mainly by the variation of intermolecular bond length whereas the intramolecular bond length remains almost unchanged. Electronic state of density was calculated to identify the bonding nature of ammonia borane. The XRD and FTIR patterns of the P42cm structure were calculated, results agree well with the experimental results of AB at room temperature.

Keywords: foundational discipline in materials science ammonia borane first－principles calculation crystal structure, hydrogen storage material

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