

研究论文

钛酸铅和钛酸钡振动性质及铁电相变的密度泛函理论研究

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摘要 采用密度泛函赝势的方法,研究了不同晶相的钛酸铅和钛酸钡的振动模式.

没有发现钛酸铅存在低温相变的证据,而钛酸钡则存在四方-正交和正交-三角铁电相变.

振动频率随四方应变的变化关系表明,随着四方应变的增大,软模的频率增大,在某一个临界点,不稳定的软模转变为稳定的振模.由于钛酸铅具有较大的四方应变,使得其能够在四方相稳定下来,而钛酸钡较小的四方应变是其仍能够发生低温铁电相变的一个重要原因.

关键词 [铁电相变](#) [振动频率](#) [四方应变](#) [钛酸铅](#) [钛酸钡](#)

分类号

A DFT Investigation of Vibrational Nature and Ferroelectric Phase Transition of BaTiO₃ and PbTiO₃

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Abstract The vibrational modes of BaTiO₃ and PbTiO₃ in different crystalline phases have been investigated by means of density functional theory pseudopotential method. No evidences of low-temperature phase transition were found for PbTiO₃, while the tetragonal-orthogonal and orthorhombic-rhombohedral phase transitions were present for BaTiO₃. The variety of vibration frequency with tetragonal strain shows that the soft mode frequency increases with the tetragonal strain increasing followed by the transition of unstable soft mode to stable vibrational mode at a certain critical point. The tetragonal phase of PbTiO₃ is very stable owing to its large tetragonal strain, and relatively small tetragonal strain of BaTiO₃ is an important reason for its low-temperature phase transition.

Key words [ferroelectric phase transition](#) [vibration frequency](#) [tetragonal strain](#) [PbTiO₃](#)- [BaTiO₃](#)

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