应用物理 电子学

(Fe$_{1-x}$N$_x$)$_4$N晶体结构和磁性的第一性　原理分析

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摘要　　运用第一性原理全势线性缀加平面波方法研究了反钙钛矿结构（Fe$_{1-x}$N$_x$)$_4$N化合物的结构和磁性质.计算了化合物晶格常数随Ni含量的变化关系；总能的计算表明镍原子优先占据角点位；结合能的计算结果显示随镍含量的增加化合物的相稳定性先上升后下降，在镍含量达到25%时化合物呈最稳定相，在镍含量大于75%后不会形成稳定相，这些结果均与实验结果一致.讨论了不同交换关联势对化合物磁矩计算结果的影响.

关键词　　FP　LAPW；铁镍氮化物；结构性质；磁性质

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Abstract

 The structural and magnetic properties of the anti　perovskite (Fe$_{1-x}$N$_x$)$_4$N compounds were investigated by employing a full potential linearized augmented plane wave method (FP　LAPW)．The dependence of lattice constants on the content of Ni was calculated．The calculated results of total energy imply that Ni prefers to occupy the corner sites rather than the face　center sites．The investigation of the dependence of the binding energy of (Fe$_{1-x}$N$_x$)$_4$N on the Ni content indicates that the stabilization of ((Fe$_{1-x}$N$_x$)$_4$N increases firstly and then decreases. The compound reaches the most stabilization at 　x=0.25　．After 　x>0.75　, it becomes unstable, which is agreed with the result of experiment very well．The effects of different exchange correlation potentials on the magnetic moment were discussed.

Key words FP　LAPW method；iron　nickel nitride；structural properties；magnetic properties

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