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CaNiN能带结构及其磁性与构型畸变关系的密度泛函 研究

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摘要 采用密度泛函方法研究了CaNiN的电子结构及其金属性和磁性，结果表明，由于弱的空间偶合作用，该化合物中一唯(1D)NiN^2-链的能带结构(Γ→X)集中反映了CaNiN的二维(2D)以及三维(3D)能带的主要特征，其能带结构揭示了CaNiN的金属性和磁性的本质，将1DNiN^2-链的结果与[MX](M=Pt,Pd,Ni;X=Cl,Br,I)对比，阐述了畸变发生的本质在于空间轨道能量的降低与核间排斥能及电子相互作用能的升高竞争的结果，发现后者占优势则不发生畸变，畸变越小越有利于材料具有顺磁性。

关键词 CaNiN 能带结构 钙化合物 镍化合物 氮化合物 磁性 畸变 密度函数 顺磁性 链结构 电子结构

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Studieson the band structures, the relationship of magnetism and distortion of CaNiN by density functional calculations

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Abstract The electronic structures of CaNiN as well as its metallic conductivity and magnetism have been studied by using DFT method. The calculated results indicate that, due to the weak interaction between the NiN^2- chains, the band structures of NiN with different dimensions are similar, which also determine the conductivity and magnetism of the compound. Compared with [MX] chains (M=Pt, Pd; X=halogen atom), it shows that the undistortion of the NiN^2- chain is mainly originated from the compertition between the decrease of the orbital energy andthe increase of the paired energy. For the [MX] chains, the latter effect is dominant and hence, the distortion of their chains is observed. It seems that the smaller distortion the compound has,the more favorable its magnetism will be.

Key words BAND STRUCTURES CALCIUM COMPOUDS NICKEL COMPOUNDS NITROGEN COMPOUNDS MAGNETISM ABERRATION PARAMAGNETISM CHAIN STRUCTURE ELECTRONIC STRUCTURE

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