AB INITIO STUDY OF MOLECULAR MAGNETISM OF m-SrN

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9.7 cm

Magnetic properties of solids typically originate in the presence of ions with partially filled d or f shells. Recently, observations of ferromagnetism in organic materials [1] and in ZnO:C [2] have stimulated interest in magnetism in systems without magnetic ions. Moreover, theory indicates that ferromagnetism can exist in II-V nitrides (SrN and CaN) in the metastable NaCl structure [3].

The experimental structure of SrN is monoclinic (m), in which there are two types of nitrogen ions with different coordinations [4]: one half on N ions form N_2 dimers, while the remaining ions are "isolated", i.e., surrounded by 6 Sr neighbors. Magnetic and electronic structure of m-SrN was analyzed within the density functional theory. We find that m-SrN is a molecular antiferromagnet. N_2 dimers are in 2- charge state with two electrons occupying antibonding π orbitals that carry magnetic moments of about 1 μ_B per dimer. The high-spin configuration of N_2 is stable because the strong exchange-induced spin polarization of the compact π orbitals dominates the relatively weak hybridization effects with Sr neighbors. Thus, this configuration is similar to that of O_2 in molecular magnet Rb_2O_6 [5].

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13.4 cm

Subject category :
2. Quantum and Classical Spin Systems

Presentation mode :
oral

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