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Electronic structure and magnetism of $Fe_{4-x}Mn_xN$ compounds
LI CHEN, Tulane University, TULANE UNIVERSITY TEAM, LINYI NORMAL UNIVERSITY TEAM — The electronic structure and magnetism of $Fe_{4-x}Mn_xN$ compounds have been studied by a periodic quantum-mechanical calculation based on density functional theory. The results show that a ferrimagnetic ordered phase is stable when Fe is substituted by Mn on cube corner sites, whereas the antiferromagnetic phase is energetically favored when Mn substitutes for Fe on face-centered sites. Mn atom concentration and the substitutional sites have significant influence on the exchange coupling. We predict covalent bonds between face-centered Fe or Mn 3d and N 2p orbitals. In contrast, bonding between the atoms at cube corners and face-centered sites is mainly ionic or metallic.

Li Chen
Tulane University

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