

Abstract Submitted  
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**Magnetic, structural and optical properties of Mn-based and Cr-based diluted magnetic semiconductors and alloys** A. ALSAAD, Jordan University of Science and Technology — We have implemented supercell approach by using local spin density functional theory for Mn-doped GaN, Mn-doped ScN and the linear muffin-tin orbital method to predict the structural and magnetic properties of these novel diluted magnetic semiconductors and their  $\text{Ga}_x\text{Mn}_{1-x}\text{N}$  and  $\text{Sc}_x\text{Mn}_{1-x}\text{N}$  alloys. The global energy minimum of MnN is obtained for zinc-blende structure. If the compound is compressed by 6 % the energy minimum corresponds to the NaCl structure in disagreement with the experimentally observed a slightly tetragonally distorted rocksalt structure, known as ? phase. The rocksalt structure of CrN at about 8 % lattice expansion becomes stable in the ferromagnetic (FM) state and has a global minimum energy at a lattice constant of 3.9 Å. We have observed an isostructural phase transition for  $\text{Sc}_x\text{Mn}_{1-x}\text{N}$  alloys from zinc-blende phase to hexagonal phase that occurs at a hydrostatic pressure of 17.5 GPa. Moreover, the structural and optical properties of single crystal CrN/ScN superlattices and  $\text{Cr}_{1-x}\text{Sc}_x\text{N}$  alloys are studied in details. We report an isostructural phase transition from wurtzite ( $w\text{-CrN}$ ) to hexagonal ( $h\text{-ScN}$ ) at a hydrostatic pressure of 21 GPa. We have also used first-principles methods to study the electronic, optical and magnetic properties of MnN and MnAs compounds in the hypothetical cubic zinc-blende phase, a phase in which the two MnN and MnAs binaries have the same local environment as that they have in GaMnN and GaMnAs alloys. We show that MnN exhibits antiferromagnetic (AFM) ground state and MnAs adopts ferromagnetic (FM) ground state.

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