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Relative stability, electronic, optical, magnetic, piezoelectric properties (Cr, Sc) N and (Mn, Sc) N alloys and CrN/ScN superlattices[1]
AHMAD ALSAAD, Jordan University of Science and Technology, Department of Physical Sciences, Irbid-Jordan, 22110 — Pure MnN, CrN binaries and their (Cr, Sc) N and (Mn, Sc) N alloys are investigated using the *ab initio* local density and generalized gradient approximation. These methods are found to predict the electronic structures, optical behavior, piezoelectric response, magnetic behavior, and relative stabilities of MnN, CrN and their $Cr_xSc_{1-x}N$ and $Mn_xSc_{1-x}N$ alloys. The magnetic configurations of MnN and CrN are studied and the results suggest that magnetic states of these compounds in zinc-blende and rocksalt phases might be more complicated than previously found by several theoretical and experimental studies. The structural stabilities of (Cr, Sc) N and (Mn, Sc) N systems were checked for the entire compositional range and crossovers from fourfold coordinated phases to sixfold coordinated phases were found at high Cr and Mn concentrations. High Curie temperature ferromagnetism in both systems was found to be possible under carefully chosen conditions. Characterization of nitride superlattices was revisited and several properties of superlattices were discussed. In particular, optical and electronic properties of CrN/ScN superlattices were studied in details.

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