Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Structural, electronic, and magnetic properties of cation mixed (Ga,Mn)(As,N) and (In,Mn)(As,N) quaternaries and (Ga,Mn)N, and (In,Mn)N ternaries AHMAD ALSAAD, ABDUALLAH SHUKRI, Jordan University of Science and Technology, DR. I.A.QATTAN, KHALIFA UNIVERSITY OF SCIENCE, TECHNOLOGY AND RESEARCH TEAM — ABINIT simulation package with local density approximation, generalized gradient approximation, and spin local density approximation have been used to investigate the structural, electronic, and magnetic properties of cation mixed (Ga,Mn)(As,N) and (In,Mn)(As,N) quaternaries contain equal and fixed compositions of Ga,In, and Mn atoms. In particular, total energy minimization approach have been used to compute the equilibrium structural parameters of zinc-blende (GaAs, InAs, and MnAs), wurtzite (GaN, InN, and MnN) binary parent compounds, as well as, the corresponding equilibrium parameters of the two (Ga,Mn)(As,N) and (In,Mn)(As,N) quaternary systems. The band structures of zince-blende GaAs, InAs and MnAs binary parent compounds have been computed and analyzed. Spin polarized band structures of the cation mixed (Ga,Mn)(As,N) and (In,Mn)(As,N) quaternaries contain equal compositions of Ga, In, and Mn cations have been computed and analyzed using spin local density approximation based calculations. Moreover, the magnetic properties of (Ga,Mn)(As,N) and (In,Mn)(As,N) quaternaries for equal concentration of Ga, In, and Mn cations have been investigated. Our simulations indicate that the two quaternary systems are nonmagnetic. This unusual result has been interpreted and explained. In addition, the magnetic properties of (Ga,Mn)N and (In,Mn)N diluted magnetic semiconductors will be presented.

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Date submitted: 17 Nov 2011 Electronic form version 1.4