Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

First-principles study of bulk MnSe and its narrow nanowires HADI AKBARZADEH, PEYMAN AMIRI, S. JAVAD HASHEMIFAR, MOHAMMAD HASSAN AMIRI, Isfahan University of Technology — Density-functional pseudo-potential calculations are employed to study the structural stability, electronic, and magnetic properties of bulk MnSe in NaCl and NiAs type structures as well as MnSe[001] nanowires in NaCl type structure. The bulk computations indicate that the LSDA+U scheme with an effective U value of about 2eV is necessary to reproduce the measured electronic and magnetic properties. Such U value is used throughout our nanowire calculations. The calculated total energies of nanowires are combined with a phenomenological model to describe the energy of broken bonds at surfaces and edges. The obtained cohesive energies are fitted by appropriate equations of state to determine the edge and surface energies of various MnAs nanowires. We conclude that occurrence of (110) facets in MnSe [001] nanowires is not favorable and rather these nanostructures prefer to have (100) and (010) facets. The significant role of edge atoms on the stability of MnSe nanowires is confirmed in all parts of our theoretical investigation.

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Date submitted: 16 Nov 2009 Electronic form version 1.4