Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

First-principles study of the iron pnictide superconductor BaFe2As2 ETHEM AKTURK, SALIM CIRACI — This work presents our study on the atomic, electronic, magnetic structures, and phonon modes of the low-temperature orthorhombic phase of undoped BaFe2As2 crystal. The electronic structure is characterized by a sharp Fe-3d peak close to the Fermi level and is dominated by Fe-3d- and As-4p-hybridized states. Ba contribution occurs only at lower energies. The spin ordering of the magnetic ground state, which is determined by minimizing the total energy of different spin alignments on Fe atoms in the conventional cell, is in agreement with experimental findings but is different from the antiferromagnetic spin ordering obtained by assigning antiparallel spin directions on two Fe atoms in the primitive unit cell. Valuable information about the charge transfer and bonding is revealed through the analysis of the charge density. Electrons are transferred from Ba to Fe-As layers and also from Fe to As atoms. The magnetic phonon calculations of the ground state are carried out to predict Raman and infrared-active modes. Softening of some calculated spin-dependent phonon modes corroborates the contribution of spin-lattice coupling to the structural phase transition from I4/mmm to Fmmm.

Ethem Akturk

Date submitted: 16 Dec 2009 Electronic form version 1.4