First Principles Calculations of the Pnictide CaFe$_2$As$_2$ under Pressure KHANDKER QUADER, Kent State University, MICHAEL WIDOM, Carnegie-Mellon University — We carry out first principles calculations of the effects of pressure on the structural and magnetic properties of the pnictide CaFe$_2$As$_2$ and compare with experiments. Our PBE-GGA calculations accurately reproduce the experimentally observed structural and magnetic ordering at zero pressure. Enthalpic considerations show that antiferromagnetic orthorhombic phase is favored over the non-magnetic tetragonal phase at pressure $P=0$, while the “collapsed” tetragonal phase is favored for pressures greater than 0.4 GPa, in good agreement with experiments. The calculated pressure dependences of the lattice parameters and the Fe-As bond lengths agree with experimental trends. We will discuss the nature of bonding and antibonding orbitals near the Fermi surface and we will evaluate the interplanar magnetic exchange interaction $J$. 

Khandker Quader
Kent State University

Date submitted: 01 Dec 2011