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First Principles Calculations of the Pnictide $CaFe_2As_2$ 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 $CaFe_2As_2$ 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.

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