Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

First principles study of uniaxial pressure-induced phase transitions in $CaFe_2As_2$ and $BaFe_2As_2$ ROSER VALENTI, MILAN TOMIC, HARALD O. JESCHKE, Institut fuer Theoretische Physik, Goethe Universitaet Frankfurt, 60438 Frankfurt, Germany — We consider density functional theory methods to determine the equilibrium structures of $CaFe_2As_2$ and $BaFe_2As_2$ under the effect of uniaxial pressure. We compare the results with calculations for hydrostatic pressure as well as with available experimental results. In $CaFe_2As_2$, we observe a unique phase transition from a magnetic orthorhombic phase to a nonmagnetic collapsed tetragonal phase for both pressure conditions and no indication of a tetragonal phase at intermediate uniaxial pressures. In contrast, for both uniaxial and hydrostatic pressure, $BaFe_2As_2$ shows two phase transitions from a magnetic orthorhombic to a collapsed tetragonal phase through an intermediate nonmagnetic tetragonal phase. We predict the critical transition pressures under uniaxial conditions to be much lower than those under hydrostatic conditions which implies that the systems are highly sensitive to uniaxial stress. We compare our results to available experimental measurements.

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Date submitted: 28 Nov 2011 Electronic form version 1.4