Effect of uniaxial stress on structural and electronic properties of \( \text{BaFe}_2\text{As}_2 \) and \( \text{CaFe}_2\text{As}_2 \)

MILAN TOMIC, HARALD O. JESCHKE, ROSER VALENTI, Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Strasse 1, 60438 Frankfurt/Main, Germany — We investigate the effects of the uniaxial tensile and compressive stresses applied along \( a \), \( b \) and \( a+b \) directions in \( \text{BaFe}_2\text{As}_2 \) and \( \text{CaFe}_2\text{As}_2 \) in the framework of ab initio density functional theory calculations. While the systems remain in the orthorhombic phase at moderate pressures, we observe an inversion of magnetism at a critical strain happening when the \( a \) and \( b \) axes approach the tetragonal condition. We discuss our results in view of recent reports of modified magnetic and structural transitions in \( \text{BaFe}_2\text{As}_2 \) under externally applied uniaxial strain and make a connection to phenomenological models proposed for these transitions.

Roser Valenti
Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Strasse 1, 60438 Frankfurt/Main, Germany

Date submitted: 27 Nov 2012
Electronic form version 1.4