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Effect of uniaxial stress on structural and electronic properties of $BaFe_2As_2$ and $CaFe_2As_2$ 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 $BaFe_2As_2$ and $CaFe_2As_2$ 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 $BaFe_2As_2$ under externally applied uniaxial strain and make a connection to phenomenological models proposed for these transitions.

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