

Abstract Submitted
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Tetragonal lattice collapse in SrFe₂As₂ - a combined experimental and theoretical study HELGE ROSNER, DEEPA KASINATHAN, MIRIAM SCHMITT, ALIM ORMECI, KATRIN MEIER, ULRICH SCHWARZ, MPI CPfS Dresden, MICHAEL HANFLAND, ESRF Grenoble, KLAUS KOEPERNIK, IFW Dresden, YURI GRIN, ANDREAS LEITHE-JASPER, MPI CPfS Dresden — In a joint experimental and theoretical study we investigate the crystal structure of the Fe pnictide compounds SrFe₂As₂ under applied hydrostatic pressure. Applying high pressure X-ray diffraction, for a critical pressure of about 10 GPa we observe a sudden collapse of the tetragonal *c* axis, accompanied by a small expansion of the basal plane. This results in a drastic reduction of the *c/a* ratio and a significant decrease of the unit cell volume. This tetragonal collapse is well described by DFT band structure calculations and can be assigned to the formation of an additional As-As bond along the tetragonal *c* axis.

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