Abstract Submitted
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Soft-mode transitions of alkaline-earth 122 pnictides[1] MICHAEL WIDOM, Carnegie Mellon University, KHANDKER QUADER, Kent State University — A-122 pnictides (A=Ca, Sr, Ba) exhibit three pressure-driven transitions: a first order enthalpic transition at P_H from the striped AFM orthorhombic (OR) to a tetragonal (T) or a collapsed tetragonal (cT) phase; a transition at $P_M > P_H$ from the metastable AFM OR to a T or cT phase; a Lifshitz transition at P_L that causes T to collapse to a cT phase. Transitions at P_H and P_L were previously examined through total energy and band structure calculations [2,3]. Here we address the transition at P_M, beyond which the metastable AFM OR state ceases to exist. We show this transition occurs through a loss of elastic stability caused by softening of a shear mode associated with stretching along the c-axis. Simultaneously, magnetism and orthorhombicity approach limiting values with an approximately square-root singularity [4]. Together these suggest a strong magneto-elastic coupling that may be relevant to a further understanding of the A-122-pnictides under pressure.

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[2]M. Widom and K. Quader, Phys. Rev. B 88, 045117 (2013)
[3]K. Quader and M. Widom, Phys. Rev. B 90, 144512 (2014)
[4]M. Widom and K. Quader, arXiv:1508.07932

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