

Abstract Submitted
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Lifshitz Transitions in 122-Pnictides Under Pressure KHANDKER QUADER, Department of Physics, Kent State University, Kent, OH 44242, MICHAEL WIDOM, Department of Physics, Carnegie-Mellon University, Pittsburgh, PA 15213 — The issue of Lifshitz transitions [1] in solids has been of considerable interest over several decades. These occur due to topological change(s) of the Fermi surface caused by external pressure or chemical substitution. Resulting anomalies in lattice parameters, density of states near the Fermi energy, elastic properties, and electron dynamics manifest in thermodynamic and transport properties that may be observed experimentally. At sufficiently high pressures, the 122 pnictides, AFe_2As_2 ($A = Ca, Sr, Ba$), display transition from a tetragonal phase (T) to a “collapsed” phase (cT). Based on our $T = 0$ first principles total energy density functional theory calculations as a function of pressure, we propose that the observed T-cT transitions result from $T = 0$ K Lifshitz transitions. Our results for energy band dispersions and spectra, c- and a-axis lattice parameters, and elastic constants over a wide range of hydrostatic pressure support our view.

[1] I. M. Lifshitz, Sov. Phys. JETP 11, 1130 (1960)

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