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Pressure-driven magnetic and structural transitions in the 122-pnictides

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Pnictides of the family AFe2As2, where A is an alkali earth element, exhibit several phase transitions in their structure and magnetic order as functions of applied pressure. We employ density functional theory total energy calculations at T=0K to model these transitions for the entire set of alkali earths (A=Ca, Sr, Ba, Ra) which form the 122 family. Three distinct types of transition occur: an enthalpic transition [1] in which the striped antiferromagnetic orthorhombic (OR-AFM) phase swaps thermodynamic stability with a competing tetragonal phase; a magnetic transition in which the OR-AFM phase loses its magnetism and orthorhombicity; a lattice parameter anomaly in which the tetragonal c-axis collapses. We identify this last transition as a "Lifshitz transition" [2] caused by a change in Fermi surface topology. Depending on the element A, the tetragonal state exhibiting the Lifshitz transition might be metastable (A=Ca) or stable (A=Sr, Ba and Ra).

[1] M. Widom and K. Quader, Phys. Rev. B 88 (2013) 045117
[2] I. M. Lifshitz, Sov. Phys. JETP 11, 1130 (1960)

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