Laboratoire des Solides Irradiés, UMR 7642

Séminaire – Mercredi 15 avril 2015 – 14H30

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Salle du laboratoire LRR (salle 05-2021)

14H00

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

Pnictides of the family AFe_2As_2, where *A* is an alkaline 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 alkaline earths (*A*=Ca, Sr, Ba, Ra) which form the 122 family. Three distinct types of transition occur: an enthalpic transition in which the striped antiferromagnetic orthorhombic (OR-AFM) phase swaps thermodynamic stability with a competing tetragonal phase; a soft-mode transition through 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" 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).