Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Density Functional Theory insights into the mechanism of non-collinear incommensurate spin density waves in Iron Arsenide. ROBERT SCHOONMAKER, STEWART CLARK, TOM LANCASTER, THOMAS FRAWLEY, PETER HATTON, Durham University — Iron arsenide intersects interesting physics between novel superconductors and other helical magnetic ordering in Pnma metal arsenide materials. Recent diffraction data has found a more complex ordering than a simple helical incommensurate spin density wave. Instead iron arsenide exhibits a definite chirality to the helimagnetism, an ellipticity in the spiral not aligned with the crystal axis, and resonant diffraction peaks forbidden by the Pnma symmetry. From non-magnetic and collinear density functional theory calculations we present insight into the mechanisms for the formation of this helimagnetic state. We find that ferromagnetic superexchange is a likely mechanism for the spin ordering and that the noncollinear ordering under this regime is caused by the spins on neighbouring irons arranging to minimise direct exchange between iron atoms, and also minimize disruption of the ferromagnetic superexchange between priveleged iron-arsenic pairs. To explain the forbidden peaks in the diffraction we have performed second-order spin-orbit perturbation calculations on the nonmagnetic calculation, which finds that the orbital ordering on the iron atoms coupled to the helimagnetism will lead to the otherwise symmetry-forbidden peaks.

Robert Schoonmaker
Durham University

Date submitted: 06 Nov 2015 Electronic form version 1.4