MS20 Electric, opto-electronic and magnetic properties from elastic and inelastic scattering plus properties of materiels from quantum crystallography

MS20-2-2 Guiding antiferromagnetic transitions in Ca_2RuO_4 #MS20-2-2

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Abstract

 Ca_2RuO_4 (CRO), the close neighbour of the famous superconductor Sr_2RuO_4 displays surprisingly different behaviour to its neighbour, exhibiting insulating behaviour below an irreversible metal-insulator transition at T_{MI} = 357K. In the insulating state CRO displays orbital ordering at T_{OO} = 260K and antiferromagnetic ordering at low temperature. Two magnetic ground states have been reported in this system with either an A-centred or B-centred order and moments predominately pointed along the b-axis. Many reports have been made altering the chemical composition of the system, including doping the atomic sites with elements of various oxidation states and atomic radii. In each case the behaviour is the same - any modification of the stoichiometric distorted structure through even low doping results in a change in magnetic ground state from the A-centred to the B-centred phase. Here we add to these results with characterisation measurements of CRO doped with manganese. We combine X-ray diffraction measurements of the crystal structure with resonant elastic X-ray scattering (REXS) measurements to determine the magnetic structure. We then use this doping regime to create a microscopic model of the system and use this to determine the nature of the transition between these two magnetic ground states. While our analysis focuses on a specific case of substitution, we show that any perturbation that can impact in a similar way on the crystal structure, by reconstructing the induced spin-orbital exchange, is able to drive the antiferromagnetic reorganization.