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Magnetic order arising from chemical chaos in A2MnRuO6 (A = Sr, Ca) double perovskites ROHAN MISHRA, PATRICK WOODWARD, WOLFGANG WINDL, The Ohio State University — Experimentally Sr_2MnRuO_6 is observed to be a c-type antiferromagnetic insulator with a tetragonal structure, while Ca_2MnRuO_6 is found to be a metallic ferrimagnet with an orthorhombic structure. Both compounds display magnetic ordering even in the absence of any recognizable chemical ordering of Mn and Ru ions. In this work, we present first principles calculations to show that the change in properties of the two compounds is only a consequence of pressure and hence can be tuned either by epitaxial growth or by alloying at A-site with Sr^{2+} or Ca^{2+} ions. We find that the Mn e_g-states are highly sensitive to pressure. Compression raises their energy in Sr_2MnRuO_6, accompanied by a transfer of electrons from the eg states to the Ru-Mn hybridized t_{2g}-states. This results in a transition from c-type antiferromagnetism to ferrimagnetism. Ferrimagnetic ordering in-turn allows for greater delocalization of the up-spin Ru t_{2g}-electrons, hence increasing the conductivity. We also show that in the presence of disorder, the Mn_{Ru} antisites couple ferromagnetically with their neighboring Mn_{Mn} sites. This allows for the interesting possibility of preserving highly spin-polarized conduction even in the absence of chemical ordering.

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