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Electron doped CrO₂: An unusual example of a charge ordered ferromagnet PRIYA MAHADEVAN, ABHINAV KUMAR, S.N. Bose National Centre for Basic Sciences, DEBRAJ CHOUDHURY, D.D. SARMA, Solid State and Structural Chemistry Unit, Indian Institute of Science — Usually metallicity accompanies ferromagnetism. K₂Cr₈O₁₆ is one of the less common examples of magnetic materials, exhibiting ferromagnetism in the insulating state [1]. Analyzing the electronic and magnetic properties within first principle electronic structure calculations, we find [2] that K acts like a donor. The doped electrons associated with the introduction of K in the lattice, induces a charge ordered and insulating ground state and interestingly also introduces a ferromagnetic coupling between the Cr ions. The primary considerations driving the charge ordering are found to be electrostatic ones with the charge being localized on two Cr atoms that minimize the electrostatic energy. The structural distortion that accompanies the ordering, generates a pathway for the electron localized on one site to hop on to the neighboring sites, a process more favorable in the ferromagnetic case, thus, giving rise to a rare example of a charge-order driven ferromagnetic insulator.

[1] Kunihiro Hasegawa *et al.*, Phys. Rev. Lett. **103**, 146403(2009).

[2] Priya Mahadevan, Abhinav Kumar, Debraj Choudhury and D.D. Sarma, Phys. Rev. Lett **104**, 256401 (2010).

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