Three Dimensional Magnetism in NaₓCoO₂

MICHELLE JOHANNES, IGOR MAZIN, Naval Research Laboratory, DAVID SINGH, Oak Ridge National Laboratory — Recent neutron studies reveal an underlying A-type antiferromagnetic order and a surprisingly three dimensional magnetism in NaₓCoO₂ for x>0.7. We look carefully at interplanar hopping in this compound, comparing supercell and virtual crystal approximation (VCA) calculations, and find that the formation of an sp² hybrid on the Na ion plays an important role in the magnetic coupling between Co ions in different layers. The specific (2b vs. 2d) position of Na ions can change the hopping integral, and therefore the superexchange, between planes indicating that Na ordering may be related to magnetic order. By reformulating a linear spin wave model to account for more than one interplanar neighbor, we show that the isotropy of magnetic interactions is due not to isotropic exchange constants but rather to the ability of each Co ion to interact with seven other Co ions in the next plane.