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Interplay of covalency and correlations in the edge shared spin 1/2 $A_3T_2O_4$ chain compounds (A = Na, K; T = Cu, Ni) DEEPA KASINATHAN, Max Planck Institute for Chemical Physics of Solids, Dresden, KLAUS KOEPERNIK, Leibniz-Institute for Solid State and Materials Research, Dresden, HELGE ROSNER, Max Planck Institute for Chemical Physics of Solids, Dresden — $Na_3Cu_2O_4$, $K_3Cu_2O_4$ and $K_3Ni_2O_4$ belong to a new class of quasi-1D insulating cuprates which feature strongly buckled, one-dimensional $^1_\infty CuO_2$ ribbon-like chains consisting of edge-sharing CuO_4 plaquettes. Structural analysis of the metal-oxygen bond lengths and thermodynamic measurements[1,2,3] imply that these systems are intrinsically charge ordered (... $(Ni/Cu)^{2+}$-$(Ni/Cu)^{3+}$-$(Ni/Cu)^{2+}$-$(Ni/Cu)^{3+}$...) and show dominant antiferromagnetic interactions. No electronic structure analysis of these systems exist to date. Using density functional theory based calculations (LDA, Wannier functions, LDA+U), we analyze the microscopic origin of the magentic interactions in these systems. The main interaction along the chains are the second neighbor superexchanges. Nonetheless, a careful analysis of the first neighbor interaction between the magnetic (Cu^{2+}/Ni^{3+}) cation and the non-magnetic cation (Cu^{3+}/Ni^{2+}) is necessary. We report on the interplay of covalency, crystal field splitting and correlations in these systems. [1] Z. Anorg. Allg.Chem. vol. 462, 92 (1980). [2] J. Solid State Chem. vol. 178, 3708 (2005). [3] Z. Anorg. Allg. Chem. vol. 637, 1101 (2011).

Deepa Kasinathan
Max Planck Institute for Chemical Physics of Solids, Dresden

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