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Formation of the one-electron structure of CoO_2 layers IGOR MAZIN, NRL, OLE ANDERSEN, MPI Stuttgart, OVE JEPSEN, MPI Stuttgart, MICHELLE JOHANNES, NRL — We use the N-order muffin tin orbital method to reduce the LDA band structure of a CoO_2 layer, the principal element of the novel superconductor $Na_xCoO_2 \cdot yH_2O$, to a three-band model and to understand it in terms of simple tight binding. We show how to introduce correctly the trigonal distortion on top of the approximately cubic local symmetry. Some of the conclusions are: (i) no adequate description of the electronic structure is possible in a one-band model and (ii) third nearest neighbor interaction appears to be important, which can be understood in terms of a superexchange via intermediate Co e_g states. We also present a set of parameters for what we believe is the minimal tight-binding model.

Igor Mazin
NRL

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