Can Electronic Structure Calculations Explain the Complex Properties of Na$_x$CoO$_2$?

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Na$_x$CoO$_2$ exhibits a remarkable variety of interesting physical properties, including charge and spin instabilities, unusual transport properties, spin-entropy driven thermoelectricity, and possibly unconventional superconductivity upon hydration. By fitting an accurate LAPW bandstructure to a tight-binding Hamiltonian, we are able to efficiently determine the doping and structural dependencies of the electronic structure of this compound. We show that, contrary to a rigid-band model, the interrelation of Na content and apical oxygen height have specific and non-negligable effects on the Fermi surface. Using an implementation of static correlation within the TB framework, we make a preliminary study of the relationship between electron localization and fermiology. We also show that the real and imaginary parts of the bare susceptibility have considerable structure in reciprocal space which is, accidentally, commensurate with the lattice. This has ramifications not only for magnetic, charge and structural instabilities, but also for the specific pairing symmetry of the superconducting state.