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Electronic Structure, Magnetism, and Superconductivity in Na_xCoO_2

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Electronic structure results for sodium cobaltate, Na_xCoO_2, and its superconducting derivative are presented. First principles calculations are used in conjunction with the tight-binding model to understand and interpret, on a microscopic level, the behaviors seen by experiment. A comparison of LDA-generated and observed optical spectra at different electron levels reveals that correlation in this system, while likely to be strong, does not manifest itself in the traditional Mott-Hubbard way. Six small Fermi surface sheets are predicted by calculation to exist at nearly all Na levels, but have not yet been seen directly by experiment. To explain the discrepancy, the calculated effects of structure change, Na level, hydration and magnetism on these pockets are presented and compared with existing experimental data. Finally, the implications of the small hole surfaces for superconductivity are explored and the presence of an exotic superconducting state is postulated.