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a_1g-e_g' splitting and the small Fermi surface pockets in Na_xCoO_2
MICHELLE JOHANNES, DEVINA PILLAY, IGOR MAZIN, Naval Research Laboratory, Washington D.C., OLE ANDERSEN, Max Planck Institute for Feskorperforshung, Stuttgart, Germany — Because DFT calculations and ARPES experiments disagree on the existence of six small Fermi surface pockets in NaxCoO2, it has been suggested that correlation effects neglected by the LDA may be responsible for suppressing the eg-derived pockets. Recent DMFT work has shown that such suppression is only possible if the position of the eg' band is lower than that of the a1g band, prior to correlation effects. Here we show that the energy difference between band positions, Δ=$\epsilon_{eg'}$-ϵ_{a1g} strongly depends on Na content, Na positions, and on whether bands stem from the surface or bulk. We show that the Coulomb field of the Na ions is enough to shift the a1g band beneath the eg band, even though simple crystal field arguments would suggest the opposite.

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