Abstract Submitted
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Does disorder destroy $e_{g'}$ pockets in $Na_{0.3}CoO_2$? A new ab initio method for disorder[1] TOM BERLIJN, DIMITRI VOLJA, WEI KU, Brookhaven National Laboratory/ Stony Brook University — Hydrated $Na_{0.3}CoO_2$ shows interesting superconductivity[1], with evidence of a nodal order parameter[2]. One possible origin of the nodal structure is *f*-wave pairing[3] due to the six $e_{g'}$ pockets predicted by the local density approximation[4]. However, ARPES experiments[5] showed no sign of these hole pockets. In this talk, we will investigate a recent proposal[6] of destruction of the $e_{g'}$ pockets due to disorder. An affordable *ab initio* Wannier function based method will be presented that takes into account spatial distributions of disorder, beyond existing mean-field approximations (e.g. VCA, CPA). We also use our Wannier functions to analyse the crystal field splitting, the sign of which critically determines the role of correlation in DMFT.

[1] K. Takada et al, Nature **422**, 53 (2003)
[2] Zheng G. et al, JPCM **18**, L63 (2006)
[3] Kuroki K. et al, PRL **93**, 077001-1 (2004)
[4] D. Singh, PRB **61**, 13397 (2000)
[5] Hasan M.Z. et al, PRL **92**, 246402 (2004)
[6] D. Singh et al PRL **97**, 016404 (2006)

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