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Effect of disorder on the electronic band structure of CaC_6: a first-principles study TOM BERLIJN, Stony Brook University/ Brookhaven National Laboratory — Recent ARPES measurements [1] raise serious questions on the Fermi surface of superconducting [2] CaC_6. Specifically, the heavily discussed Ca band was not observed, and the charge transfer from Ca is found largely complete, contrary to previous theoretical studies [3-6]. Here we investigate the effects of potential Ca disorder on the electronic band structure, using a newly developed Wannier function-based disorder method. In particular, quasi-localization of the Ca carriers will be examined via the one-particle spectral function.

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