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Layer Dependence of Charge Distribution and Electronic Structure of $\text{HgBa}_2\text{Ca}_4\text{Cu}_5\text{O}_{12}$ WEI-GUO YIN, DMITRI VOLJA, WEI KU, Brookhaven National Laboratory, WARREN PICKETT, University of California, Davis, DEEPA KASINATHAN, Max-Planck Institute for Chemical Physics of Solids — Recent experimental observation of layer-dependent properties of the five-layer superconducting cuprate $\text{HgBa}_2\text{Ca}_4\text{Cu}_5\text{O}_{12+\delta}$ has inspired intensive interest. In general, multi-layer cuprates are of great interest because the influence of the apical oxygen p states, the main source of the material dependence of cuprate structural and electronic properties [1], could be significantly layer-dependent. In this talk, the layer dependence of the charge distribution and electronic structure of $\text{HgBa}_2\text{Ca}_4\text{Cu}_5\text{O}_{12}$ will be investigated via the recently developed many-body Wannier-state method [1]. Possible implications on modulation of local pairing gaps, hole mobility, “super-repulsion” [1], and electron-phonon interaction among these distinct CuO_2 layers will be discussed, in connection with the intriguing experimental findings of coexisting superconducting and antiferromagnetic orders as well as strong interlayer charge inhomogeneity. Work partially supported by DOE-CMSN. [1] W.-G. Yin and W. Ku, cond-mat/0702469.

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