Quasiparticle self-consistent GW study of cuprates: electronic structure, model parameters, and the two-band theory for Tc

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An important open question for high-Tc cuprates is about the material dependence of the superconducting properties. Using the quasiparticle self-consistent GW (QSGW) method, we re-examine the electronic structure of the parent compounds of copper oxide high-Tc materials. We show that QSGW captures several important features, distinctive from the conventional LDA results. The energy level splitting between dx2-y2 and d3z2-r2 is significantly enlarged and the van Hove singularity point is lowered. The calculated results compare better than LDA with recent experimental results from resonant inelastic xray scattering and angle resolved photoemission experiments. This agreement with the experiments supports the previously suggested two-band theory for the material dependence of the superconducting transition temperature, Tc.