

Figure 2: Wannier-like orbital for the conduction band of the high temperature superconductor $HgBa_2CuO_4$, plotted in the CuO_2 -plane. This orbital has $Cu\ d_{x^2-y^2}$ symmetry and extends over several neighboring oxygen (*) and copper (+) sites. It was computed with the third-generation linear muffin-tin orbital (LMTO) method, using the local density approximation (LDA).