Cu OAO occupations Nup+Ndown Nup-Ndown 2.0 0.5 1.8 1.6 0.0 1.4 1.2 -0.51.0 8.0 3dxy 3dyz 38 3pz 3dxy 3dyz 38 **4**s 3px 3py 3pz 4s 3dxz 3px 3py