Cu OAO occupations Nup+Ndown Nup-Ndown 2.0 0.5 1.8 1.6 1.4 0.0 1.2 1.0 -0.50.8 0.6 38 **4**s 3dxy 3dyz 3dz^2 3dxz 3s 4s 3px 3py 3pz 3dxy 3dxy 3px 3py 3pz