Cu OAO occupations Nup+Ndown Nup-Ndown 2.0 0.4 1.8 0.2 1.6 0.0 1.4 -0.21.2 -0.41.0 3s 3dxy 3dyz 3dz^2 3dxz **4**s 38 4s 3px 3py 3dxy 3dyz 3px 3py 3pz 3pz