Cu OAO occupations Nup+Ndown Nup-Ndown 2.0 0.6 1.8 0.4 1.6 0.2 1.4 0.0 1.2 -0.2-0.41.0 -0.68.0 -0.83s 3pz 3dxy 3s 4s 3dyz 3dxz 4s 3px 3py 3px 3py 3pz 3dxy 3dyz