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 3px 3py 3pz 3dxy 3s 3dxz 3s 3px 3py 3pz 3dxy 3dyz 4s 4s 3dyz