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 -0.21.0 -0.40.8 -0.60.6 -0.83pz 3dxy 3dyz 38 4s 3dxz 38 4s 3px 3py 3pz 3px 3py 3dyz 3dxy