Cu OAO occupations Nup+Ndown Nup-Ndown 0.4 2.0 0.2 1.8 0.0 1.6 1.4 -0.21.2 -0.41.0 -0.60.8 -0.83dxy 3dyz 3s 4s 38 **4**s 3px 3py 3pz 3dz^2 3dxz 3px 3py 3pz 3dxy 3dyz