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 1.0 -0.20.8 -0.40.6 3pz 3dxy 38 38 4s 3dxz 4s Зрх 3pz 3dxy 3dyz 3px 3py Зру 3dyz