Cu OAO occupations Nup+Ndown Nup-Ndown 0.5 0.1 0.0 0.4 0.3 -0.10.2 -0.20.1 -0.30.0 -0.4-0.1-0.53dyz 3dxz 38 4s 3ру 3рz 3dz^2 38 4s 3dxy 3dyz Зрх 3px 3py 3pz 3dxy