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 -0.6-0.80.6 3s 4s 3pz 3dxy 3dxz 3s 4s 3dyz 3dz^2 3dxy 3dyz Зрх Зру 3px 3py 3pz