Cu IAO 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 3pz 3dxy 3dyz 3dz^2 3dxz 3s 3px 3py 3pz 3dxy 3dxy 38 4s 4s Зрх Зру