Cu OAO occupations Nup+Ndown Nup-Ndown 0.2 -0.40.0 -0.5-0.2-0.6-0.4-0.7-0.6-0.8-0.8-0.9-1.0-1.0-1.23dxz 2-y^2 3s 4s 3px 3py 3pz 3dxy 3dxy 38 **4**s 3dxy 3dyz Зрх 3py 3pz