Cu IAO2 occupation diff:ACHN2-ACHN Nup+Ndown Nup-Ndown 0.3 0.05 0.00 0.2 -0.05 -0.10 0.1 -0.15 -0.20 0.0 0.25 0.30 -0.13dxz 38 **4**s 3dxy 3dyz 4s 3dxy 3dyz 3px 3py 3pz Зрх 3pz 38 Зру