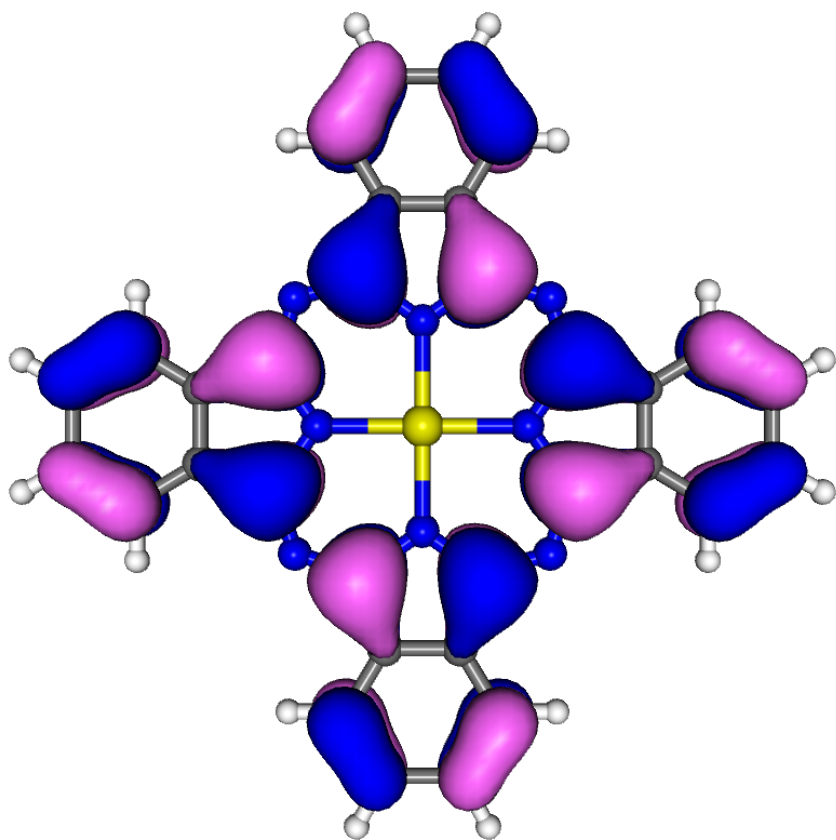
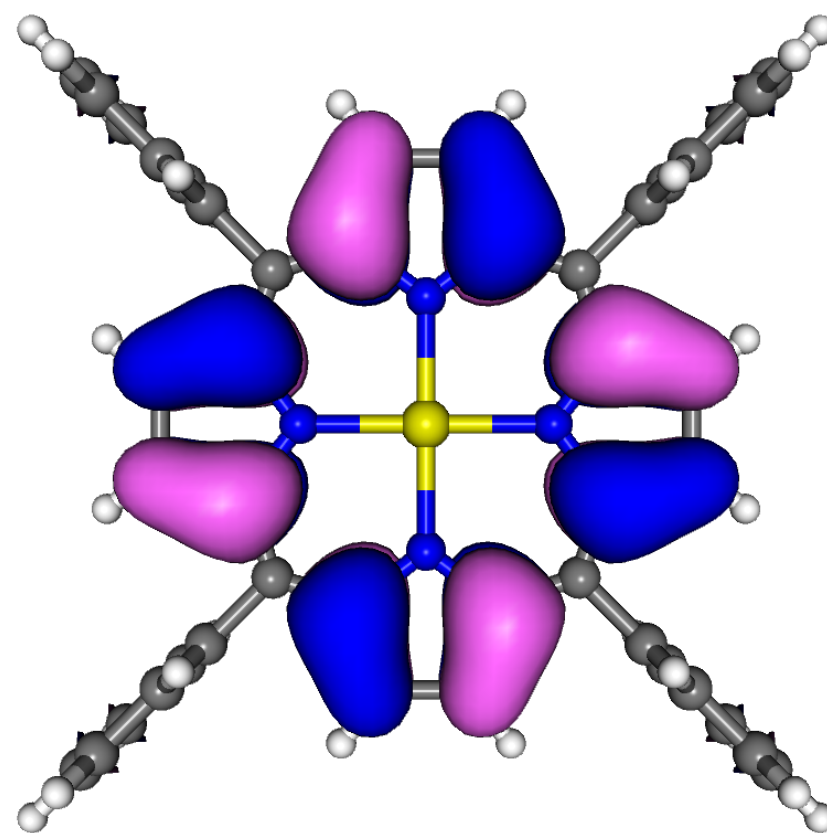


$2a_{1u}$ MO



CuPc



CuTPP

Figure S2. 3D contour plot of the CuPc and CuTPP $2a_{1u}$ MO. Displayed isosurfaces correspond to $\pm 0.02 e^{1/2} \text{Å}^{-3/2}$ values