



Figure S1. 3D contour plots of the  $N^{Py}$ -based  $Pc^{2-}$  and  $TPP^{2-}$  frontier  $\pi$  and  $\sigma$  MOs. Displayed isosurfaces correspond to  $\pm 0.02 e^{1/2} \text{ \AA}^{-3/2}$  values