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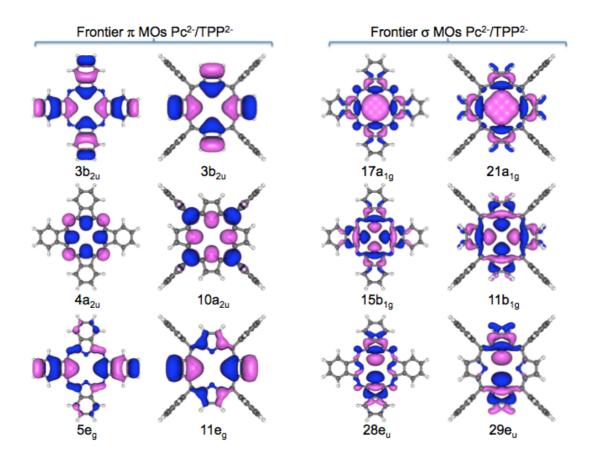


Figure S1. 3D contour plots of the N^{Py}-based Pc²⁻ and TPP²⁻ frontier π and σ MOs. Displayed isosurfaces correspond to ±0.02 e^{1/2} Å^{-3/2} values