

Supporting Information:

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FIG. 1: Plots of the electron localisation function (ELF) along planes bisecting four of the expanded atom species.

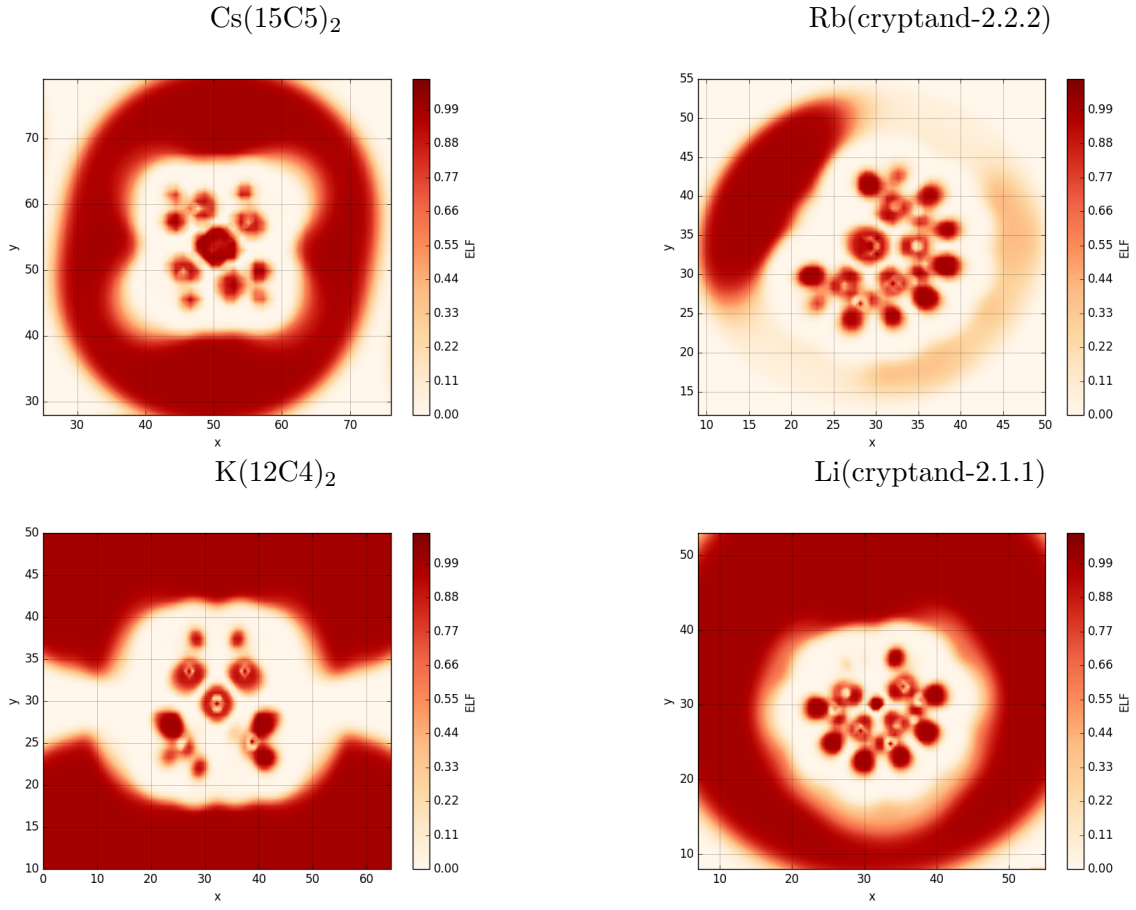


FIG. 2: Highest occupied molecular orbital (HOMO) densities for four of the expanded atoms, plotted using a 0.1 a.u. isosurface.

