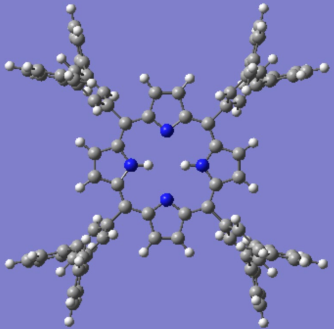
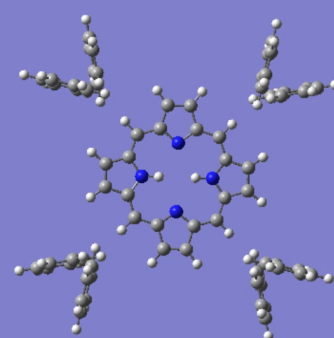
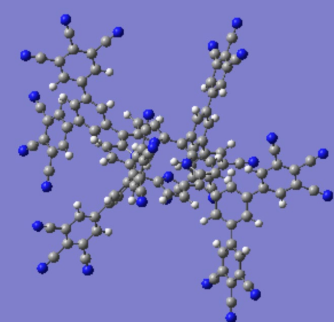
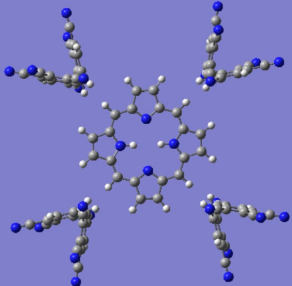
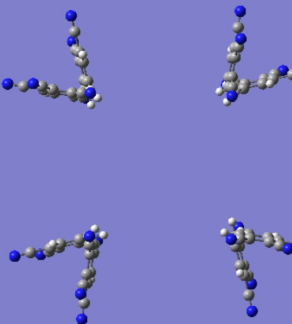
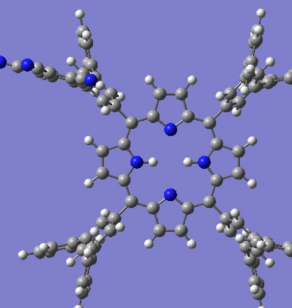
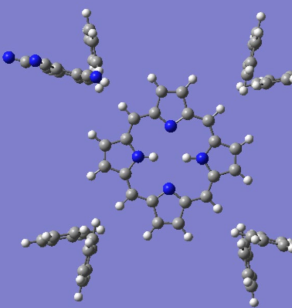
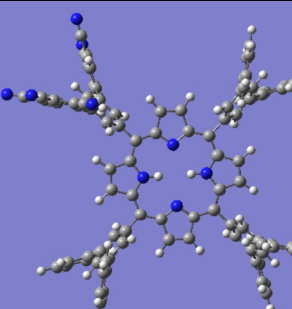


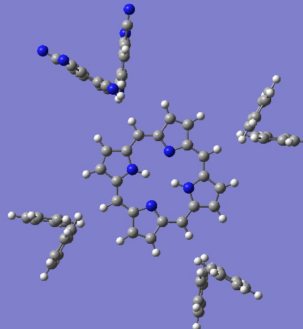
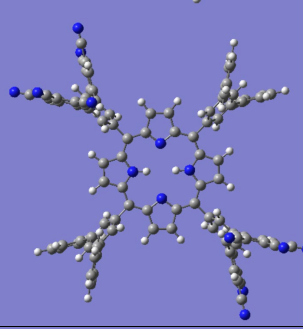
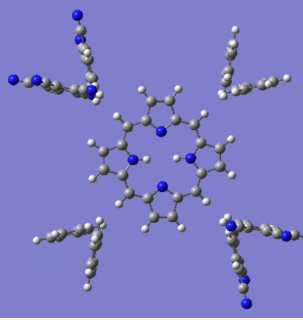
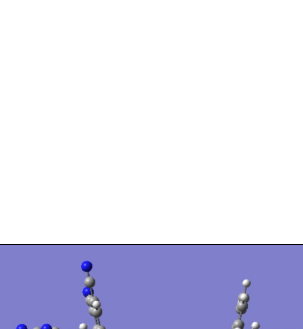
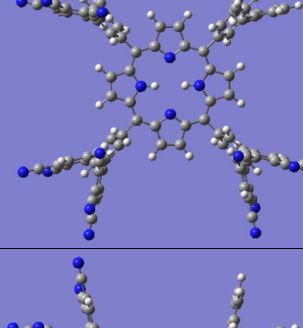
The character of simulations is explained the first time they appear in this document

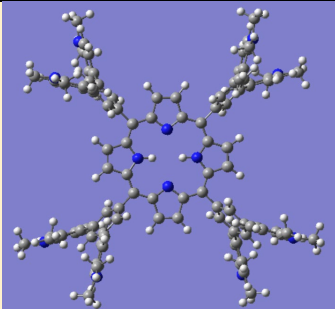
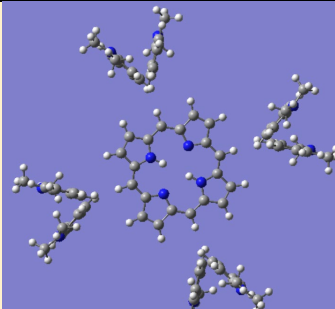
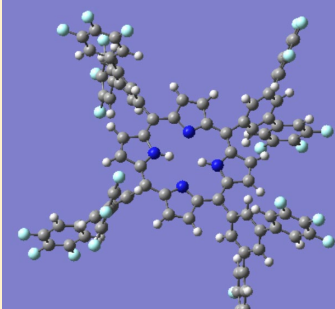
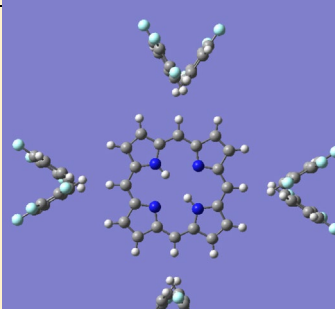
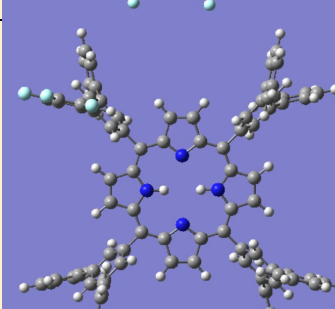
In addition to the files listed in the table below, the repository contains also additional simulations (apart from the per-/suffix the names follow the same logic as the listed files):

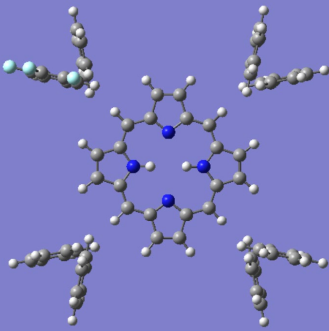
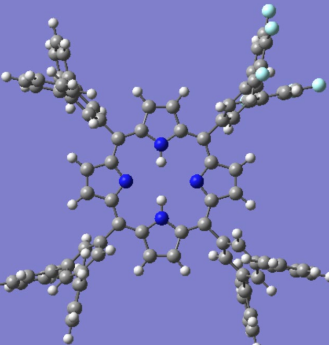
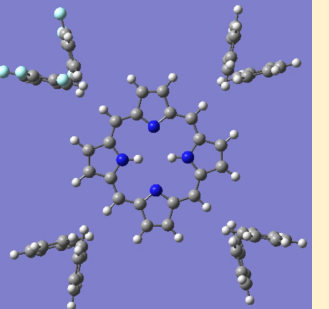
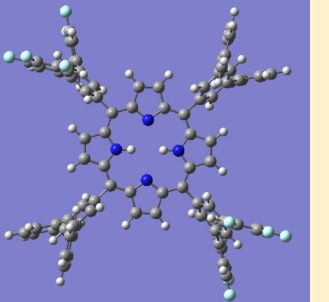
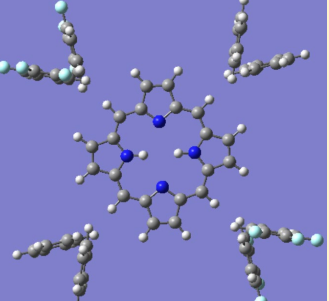
- files with the suffix “-Hirsh” are the ones used for calculating Hirschfeld charges. They are contained in the subfolder /Hirshfeld
- files with a prefix “D-” correspond to simulations including the Grimme D3 correction. They are contained in the subfolder /Grimme
- files contained in the subfolder *adiabatic* that do not contain the element “dif1” are geometry optimizations of cations and anions performed with the 6-31G(d,p) basis set; files in that folder containing “dif1” are single points where those containing “+SP+” are calculations cations using the cation geometry and those containing “--SP-” are calculations of anions using the anion geometry.
- The folder called *porph* contains reference simulations of a porphyrin molecule. The naming convention follows the same logic as for the larger molecules: *porph-gjf* is a geometry optimization of the neutral molecule with the smaller basis set; +/- refers to cations and anions, where a single – in the middle of a filename can also be a hyphen; *dif1* indicates the use of the larger basis set; all calculations containing the term “SP” are single-point calculations and all calculations not containing “SP” are geometry optimizations

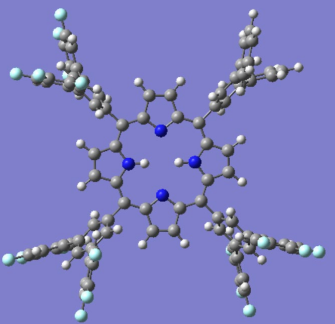
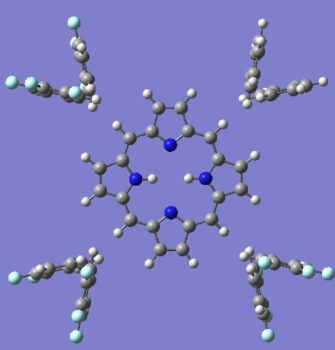
		geometry optimization (6-31G(d,p)) porph-b2g single point neutral (6-311+G(d,p)) diffuse/porph-b2g-SPdif1, single point cation (6-311+G(d,p)) diffuse/porph-b2g-SP+dif1, single point anion (6-311+G(d,p)) diffuse/porph-b2g-SP-dif1
		system with removed bridging benzenes: take output geometry from porph-b2g, remove bridging benzenes, saturate by H and only positions of those H atoms. porphX-b2g diffuse/porphX-b2g-SPdif1, diffuse/porphX-b2g-SP+dif1, diffuse/porphX-b2g-SP-dif1
		porph-b2g-CNa-max diffuse/porph-b2g-CNa-max-SPdif1, diffuse/ porph-b2g-CNa-max-SP+dif1, diffuse/ porph-b2g-CNa-max-SP-dif1

		porphX-b2g-CNa-max diffuse/ porphX-b2g-CNa-max-SPdif1, diffuse/ porphX-b2g-CNa-max-SP+dif1, diffuse/ porphX-b2g-CNa-max-SP-dif1
		porphY-b2g-CNa-max-SPdif1 start from porphX-b2g-CNa-max geometry and remove porphyrin
		CN-groups only on 1 ring porph-b2g-CNa1-max diffuse/porph-b2g-CNa1-max-SPdif1, diffuse/porph-b2g-CNa1-max-SP+dif1, diffuse/porph-b2g-CNa1-max-SP-dif1
		porphX-b2g-CNa1-max diffuse/porphX-b2g-CNa1-max-SPdif1, diffuse/porphX-b2g-CNa1-max-SP+dif1, diffuse/porphX-b2g-CNa1-max-SP-dif1 diffuse/porphY-b2g-CNa1-max-SPdif1
		CN-groups only on 2 rings porph-b2g-CNa2-max diffuse/porph-b2g-CNa2-max-SPdif1, diffuse/ porph-b2g-CNa2-max-SP+dif1, diffuse/ porph-b2g-CNa2-max-SP-dif1

		porphX-b2g-CNa2-max diffuse/porphX-b2g-CNa2-max-SPdif1, diffuse/porphX-b2g-CNa2-max-SP+dif1, diffuse/porphX-b2g-CNa2-max-SP-dif1 diffuse/porphY-b2g-CNa2-max-SPdif1
		porph-b2g-CNa4-max diffuse/porph-b2g-CNa4-max-SPdif1, diffuse/porph-b2g-CNa4-max-SP+dif1, diffuse/porph-b2g-CNa4-max-SP-dif1
		porphX-b2g-CNa4-max diffuse/porphX-b2g-CNa4-max-SPdif1, diffuse/porphX-b2g-CNa4-max-SP+dif1, diffuse/porphX-b2g-CNa4-max-SP-dif1 diffuse/porphY-b2g-CNa4-max-SPdif1 problematic case: calculate without diffuse: diffuse/porphX-b2g-CNa4-max-SP+ read guess from checkpoint then with diffuse: diffuse/porphX-b2g-CNa4-max-SP+dif1a still did not work ... try other intermediate step: 6-31+G(d,p) basis as intermediate step diffuse/porphX-b2g-CNa4-max-SP+dif1x (converged) then use guess=read based on the converged density of that calculation for a 6-311+G(d,p) basis: diffuse/porphX-b2g-CNa4-max-SP+dif1y
		porph-b2g-CNa6-max diffuse/porph-b2g-CNa6-max-SPdif1, diffuse/porph-b2g-CNa6-max-SP+dif1, diffuse/porph-b2g-CNa6-max-SP-dif1
		porphX-b2g-CNa6-max diffuse/porphX-b2g-CNa6-max-SPdif1, diffuse/porphX-b2g-CNa6-max-SP+dif1, diffuse/porphX-b2g-CNa6-max-SP-dif1 diffuse/porphY-b2g-CNa6-max-SPdif1 problematic case: calculate without diffuse: diffuse/porphX-b2g-CNa6-max-SP+ read guess from checkpoint then with diffuse:

		diffuse/porphX-b2g-CNa6-max-SP+dif1a
		porph-b2g-DMA (build on reference geometry, have all pyramides on one side of the porphyrin point in the same direction and on the other side in the other ...) geometry not converged after 12h restart with longer time limit. porph-b2g-DMAcont diffuse/porph-b2g-DMA-SPdif1, diffuse/porph-b2g-DMA-SP+dif1, diffuse/porph-b2g-DMA-SP-dif1 problematic case: calculate without diffuse: diffuse/porphX-b2g-DMA-SP+ read guess from checkpoint then with diffuse: diffuse/porphX-b2g-DMA-SP+dif1a
		porphX-b2g-DMA diffuse/porphX-b2g-DMA-SPdif1, diffuse/porphX-b2g-DMA-SP+dif1, diffuse/porphX-b2g-DMA-SP-dif1 diffuse/porphY-b2g-DMA
		porph-b2g-Fa-max0 diffuse/porph-b2g-Fa-max0-SPdif1, diffuse/porph-b2g-Fa-max0-SP+dif1, diffuse/porph-b2g-Fa-max0-SP-dif1
		porphX-b2g-Fa-max0 diffuse/porphX-b2g-Fa-max0-SPdif1, diffuse/porphX-b2g-Fa-max0-SP+dif1, diffuse/porphX-b2g-Fa-max0-SP-dif1 porphY- b2g-Fa-max0
		porph-b2g-Fa1-max0 same rings as for CN system! diffuse/porph-b2g-Fa1-max0-SPdif1, diffuse/porph-b2g-Fa1-max0-SP+dif1, diffuse/porph-b2g-Fa1-max0-SP-dif1

		porphX-b2g-Fa1-max0 diffuse/porphX-b2g-Fa1-max0-SPdif1, diffuse/porphX-b2g-Fa1-max0-SP+dif1, diffuse/porphX-b2g-Fa1-max0-SP-dif1 no porphyrine diffuse/porphY-b2g-Fa1-max0-SPdif1
		porph-b2g-Fa2-max0 same rings as for CN system! diffuse/porph-b2g-Fa2-max0-SPdif1, diffuse/porph-b2g-Fa2-max0-SP+dif1, diffuse/porph-b2g-Fa2-max0-SP-dif1
		porphX-b2g-Fa2-max0 diffuse/porphX-b2g-Fa2-max0-SPdif1, diffuse/porphX-b2g-Fa2-max0-SP+dif1, diffuse/porphX-b2g-Fa2-max0-SP-dif1 no porphyrine diffuse/porphY-b2g-Fa2-max0-SPdif1
		porph-b2g-Fa4-max0 same rings as for CN system! diffuse/porph-b2g-Fa4-max0-SPdif1, diffuse/porph-b2g-Fa4-max0-SP+dif1, diffuse/porph-b2g-Fa4-max0-SP-dif1
		porphX-b2g-Fa4-max0 diffuse/porphX-b2g-Fa4-max0-SPdif1, diffuse/porphX-b2g-Fa4-max0-SP+dif1, diffuse/porphX-b2g-Fa4-max0-SP-dif1 no porphyrine diffuse/porphY-b2g-Fa4-max0-SPdif1

	porph-b2g-Fa6-max0 same rings as for CN system! diffuse/porph-b2g-Fa6-max0-SPdif1, diffuse/porph-b2g-Fa6-max0-SP+dif1, diffuse/porph-b2g-Fa6-max0-SP-dif1
	porphX-b2g-Fa6-max0 diffuse/porphX-b2g-Fa6-max0-SPdif1, diffuse/porphX-b2g-Fa6-max0-SP+dif1, diffuse/porphX-b2g-Fa6-max0-SP-dif1 no porphyrine diffuse/porphY-b2g-Fa6-max0-SPdif1

Some info regarding exemplary cube files

cubegen 1 MO=HOMO porph-b2g-CNa-max-SPdif1.fchk porph-b2g-CNa-max-SPdif1-HOMO.cub -3

cubegen 1 potential porphY-b2g-CNa-max-SPdif1.fchk porphY-b2g-CNa-max-SPdif1.cub -3

Charge-density differences:

porph-b2g-CNa-max-SP-dif1-dens-diff.cub = porph-b2g-CNa-max-SP-dif1-density.cub - porph-b2g-CNa-max-SPdif1-density.cub