

[1/1] ML_ABN (LaMnO3:)

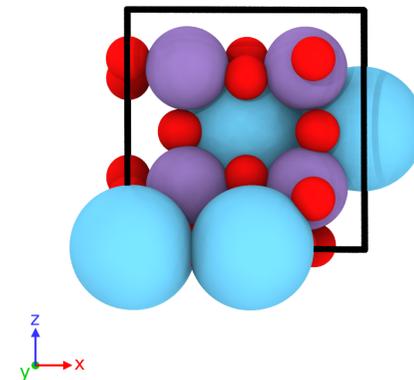
file

name ML_ABN
 structure groups 1
 total structures 577

overview

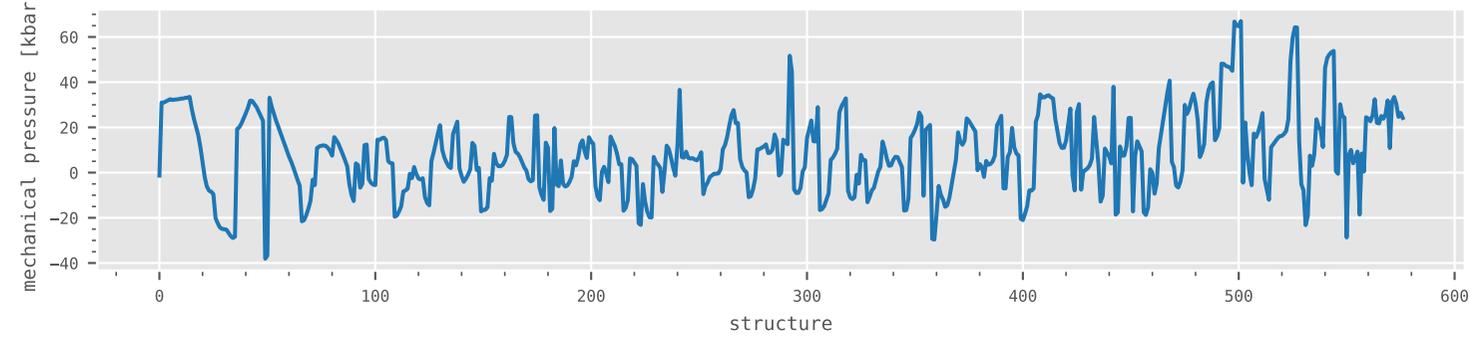
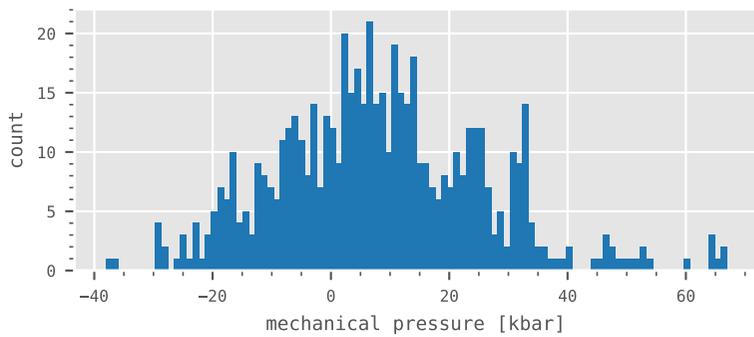
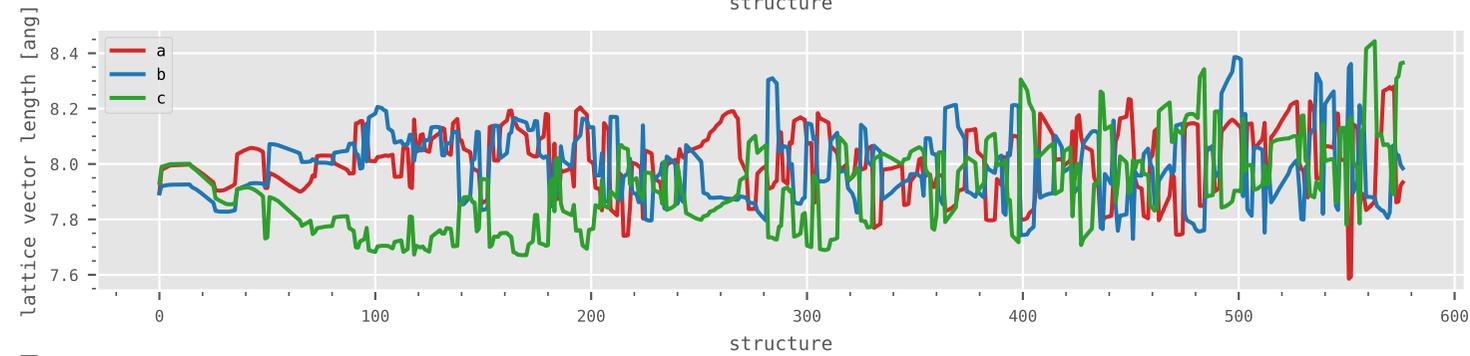
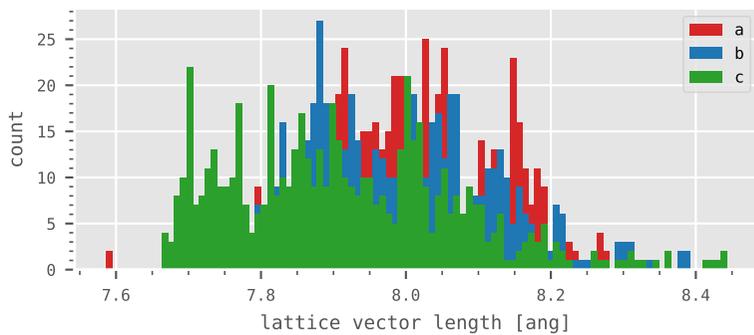
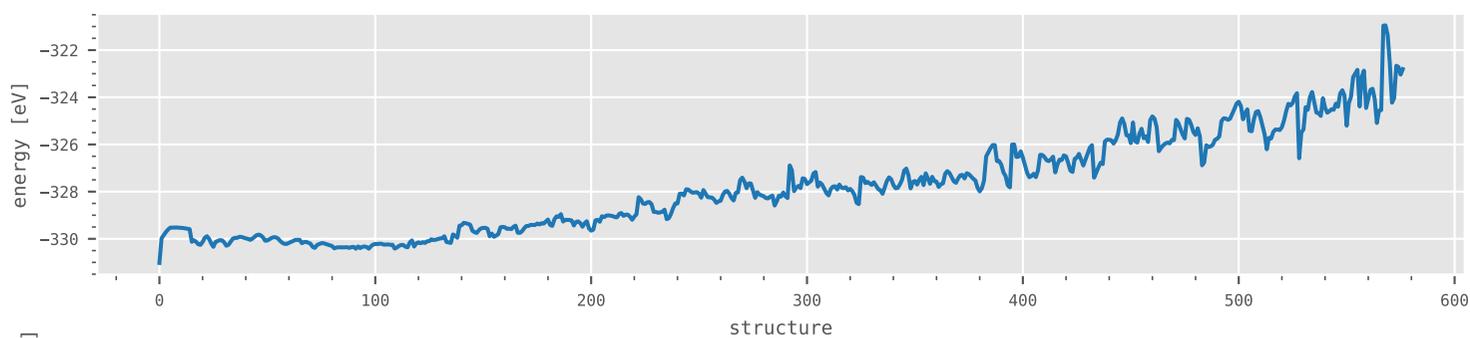
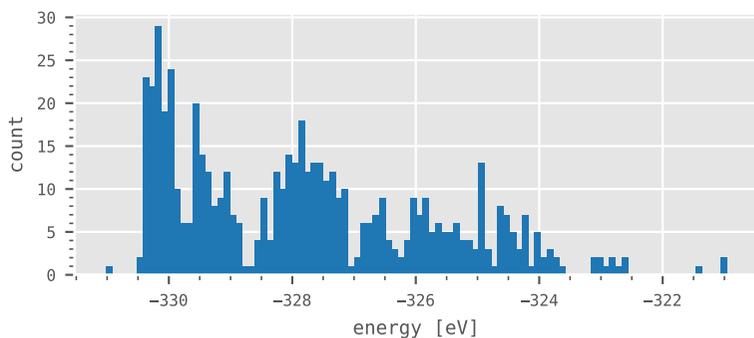
energy -327.8 ± 2.06 eV
 volume 506.7 ± 9.25 ang³
 lattice vector a 8.0 ± 0.12 ang
 lattice vector b 8.0 ± 0.13 ang
 lattice vector c 7.9 ± 0.16 ang
 non-periodic radius 3.8 (min. for group) ang

min energy configuration



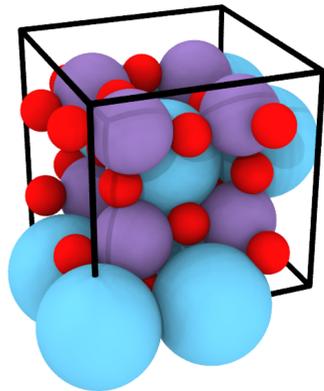
current structure group

name LaMnO3:
 structure group 1 (of 1 in file)
 structures 577 (of 577 in file)
 atoms La (8), Mn (8), O (24)
 40 total

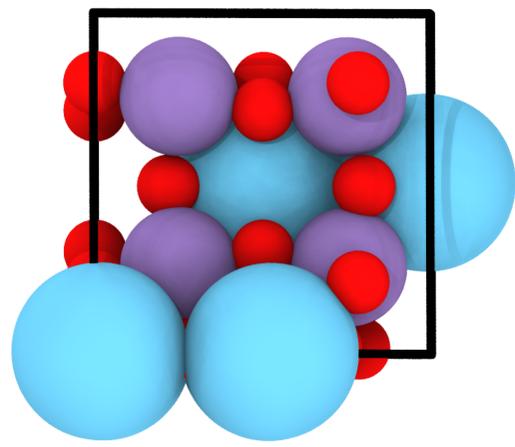


minimum energy configuration (structure 1)

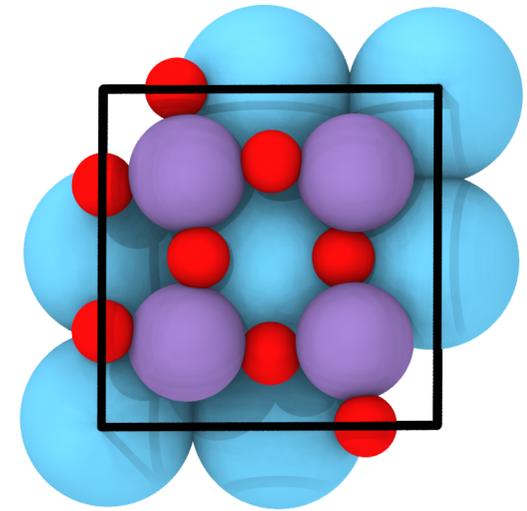
perspective



front

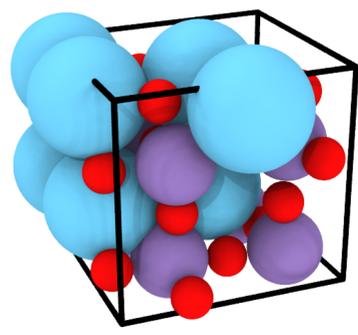


top

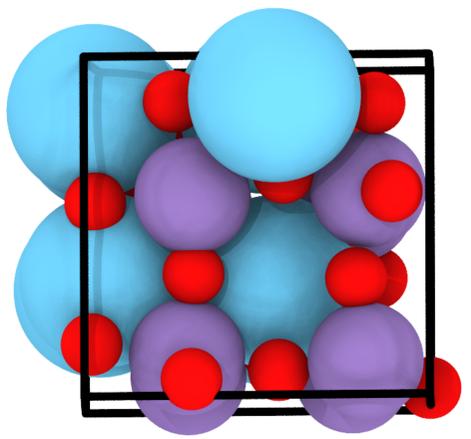


maximum energy configuration (structure 569)

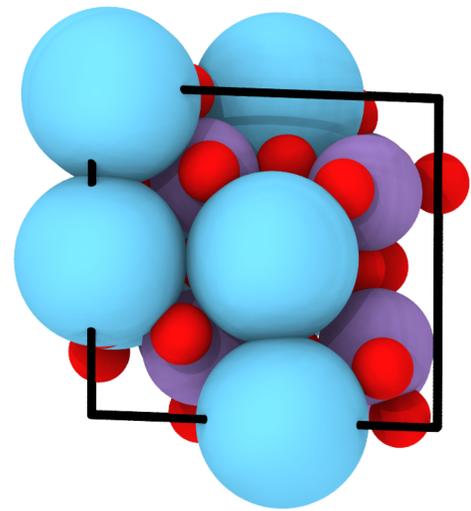
perspective



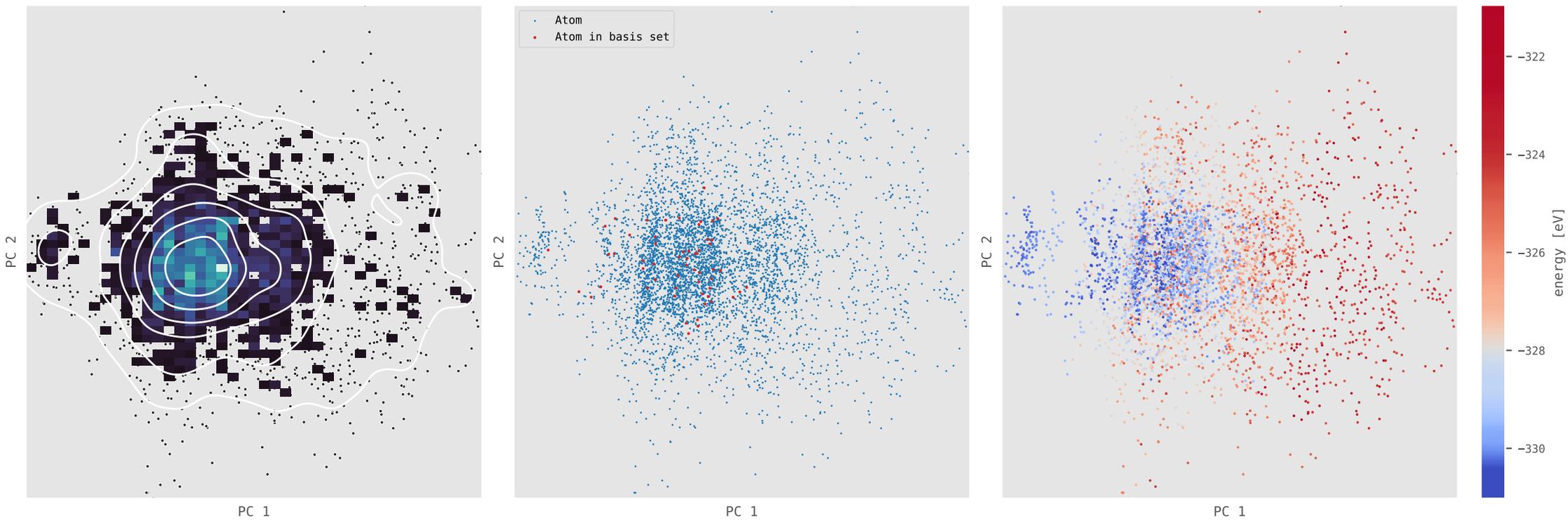
front



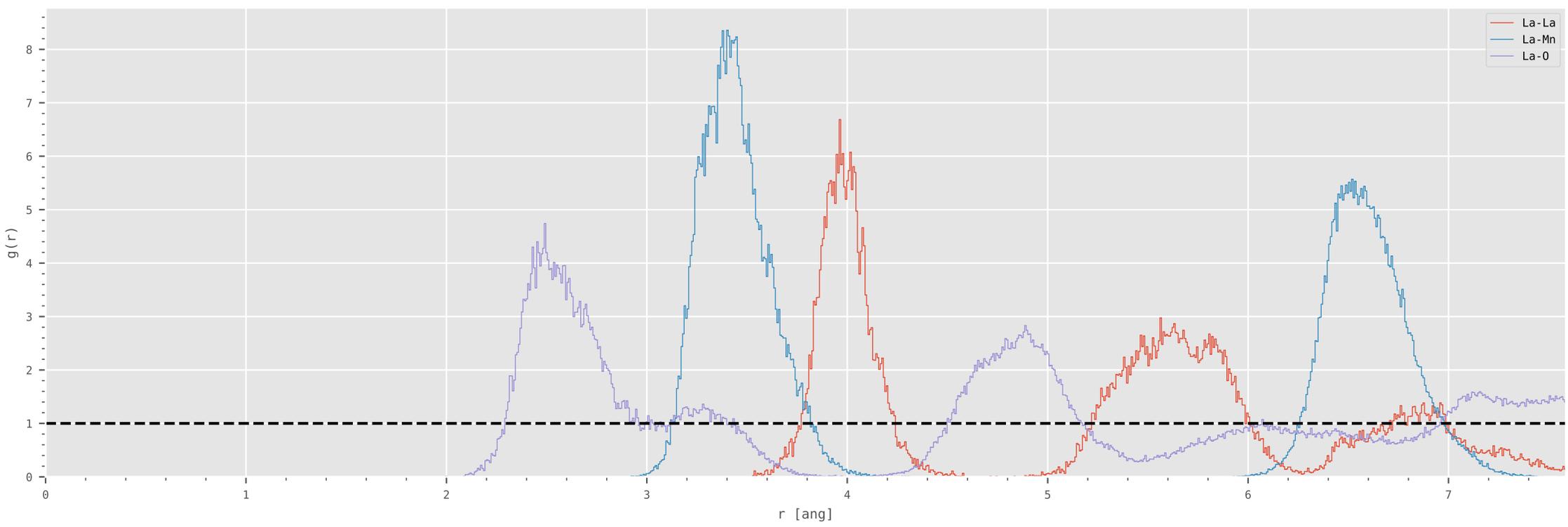
top



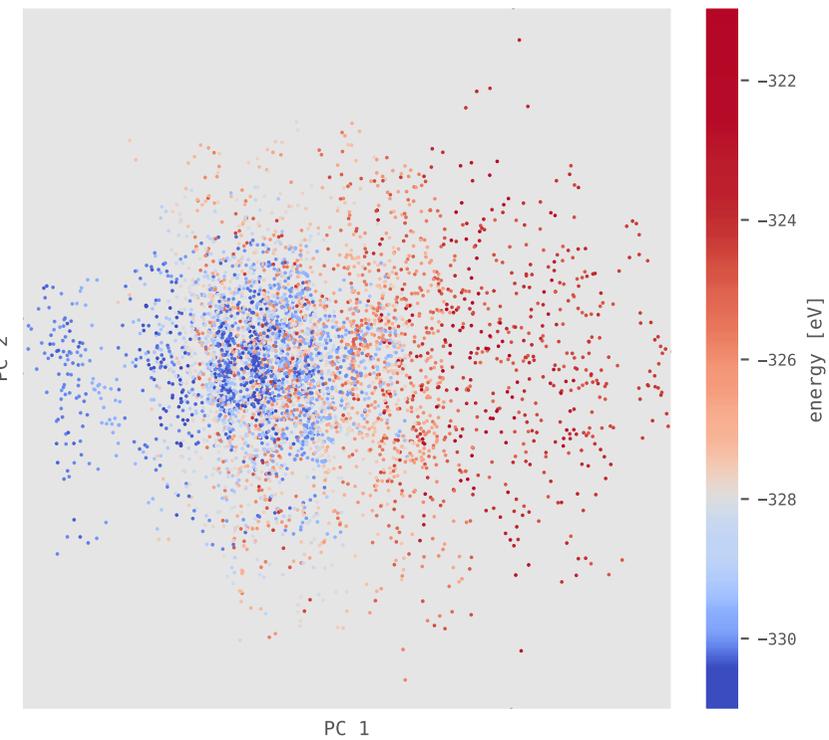
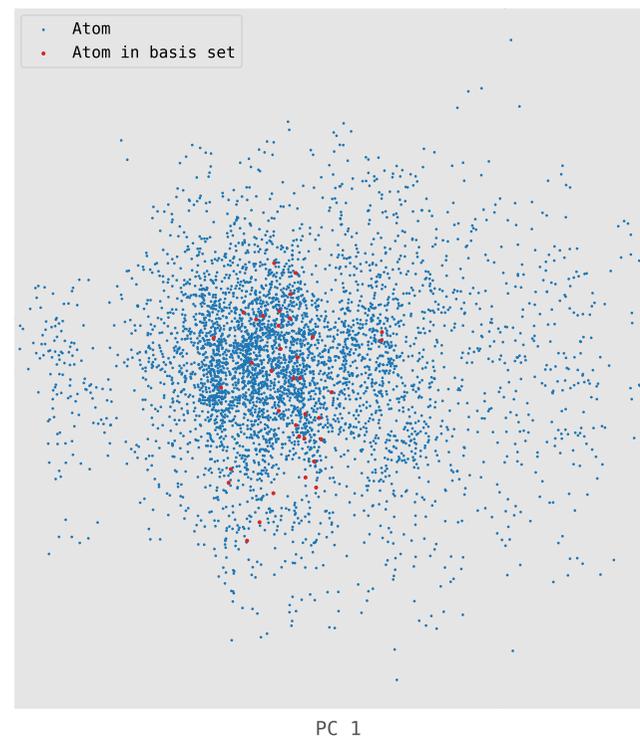
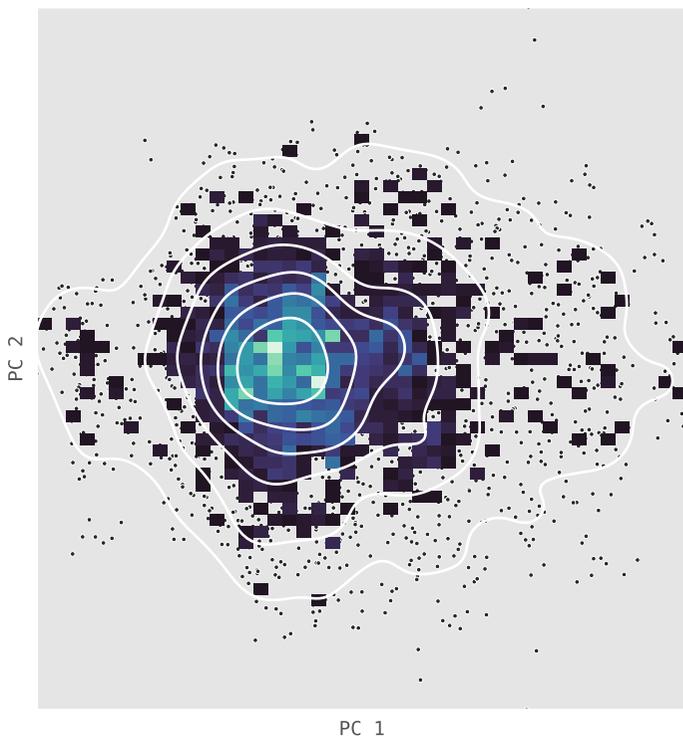
principal component analysis of descriptors (La)



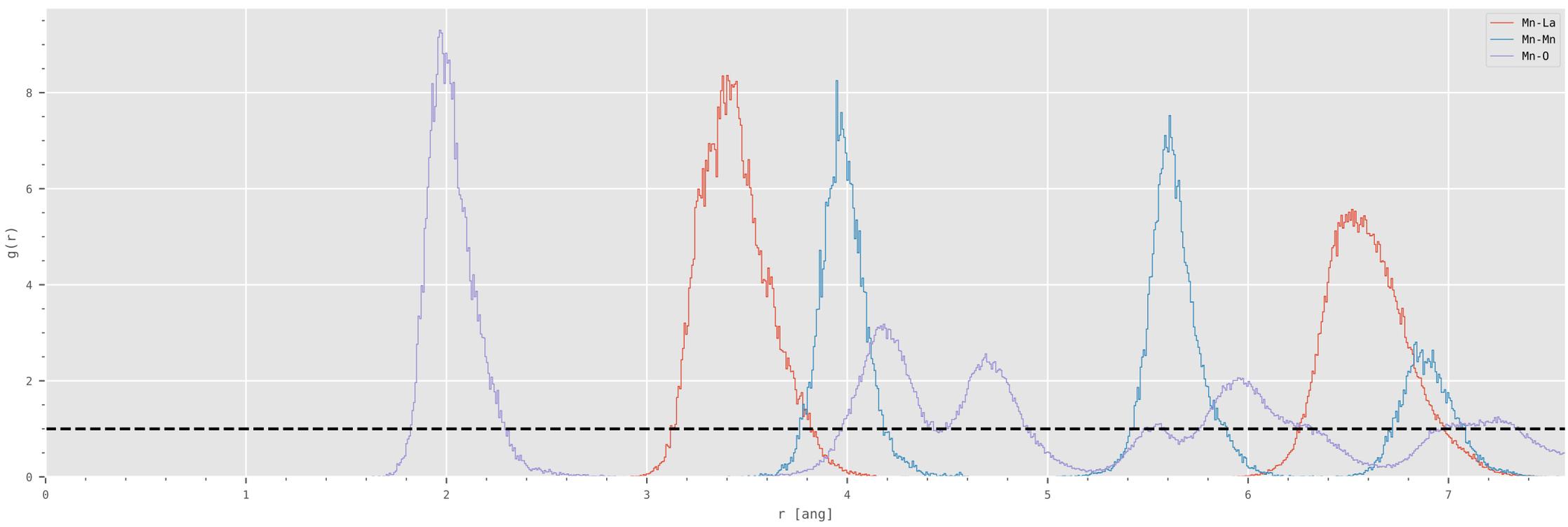
radial distribution functions (La)



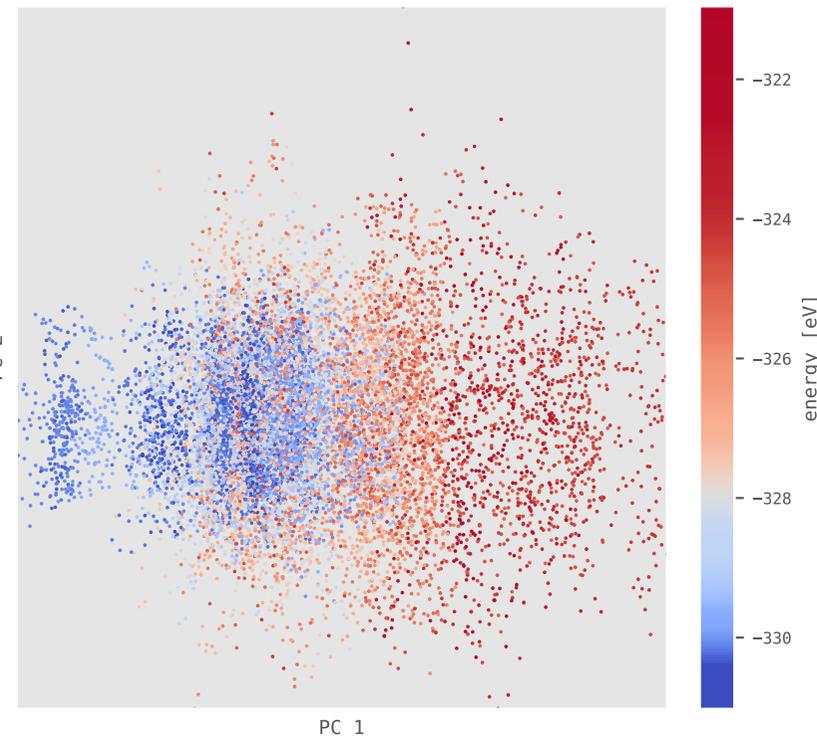
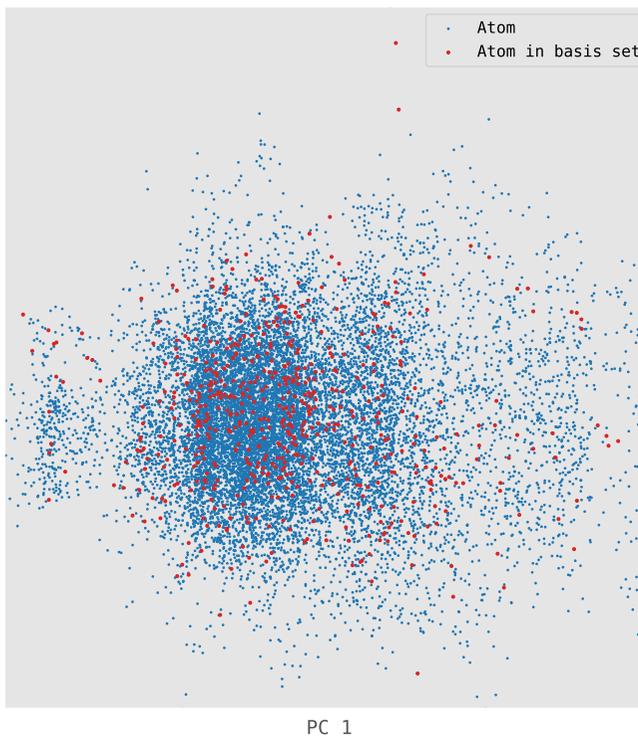
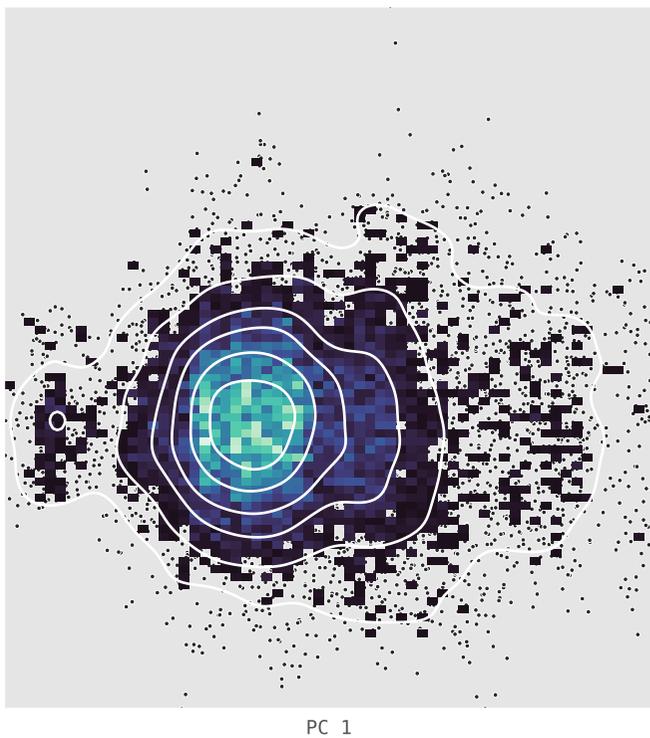
principal component analysis of descriptors (Mn)



radial distribution functions (Mn)



principal component analysis of descriptors (0)



radial distribution functions (0)

