[1/1] ML_AB_heavymass (CsPbBr3 Cubic MLFF 400 K)

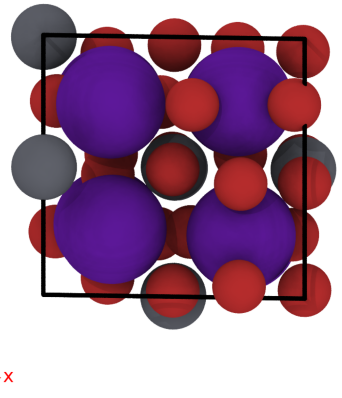
file

name	ML_AB_heavymass
structure groups	1
total structures	639

overview

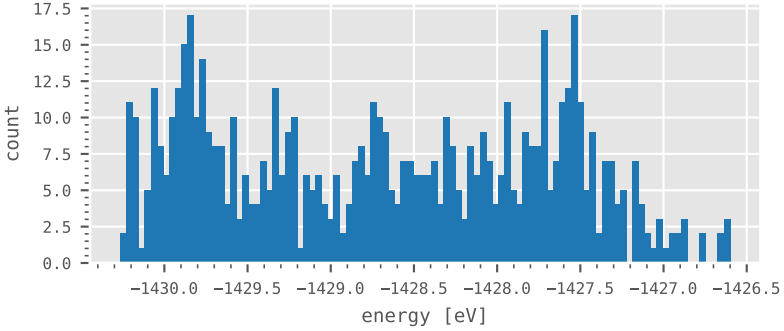
energy	-1428.7 ± 0.97	eV
volume	1659.2 ± 36.83	ang^3
lattice vector a	11.8 ± 0.15	ang
lattice vector b	11.9 ± 0.15	ang
lattice vector c	11.8 ± 0.18	ang
non-periodic radius	5.7 (min. for group)	ang

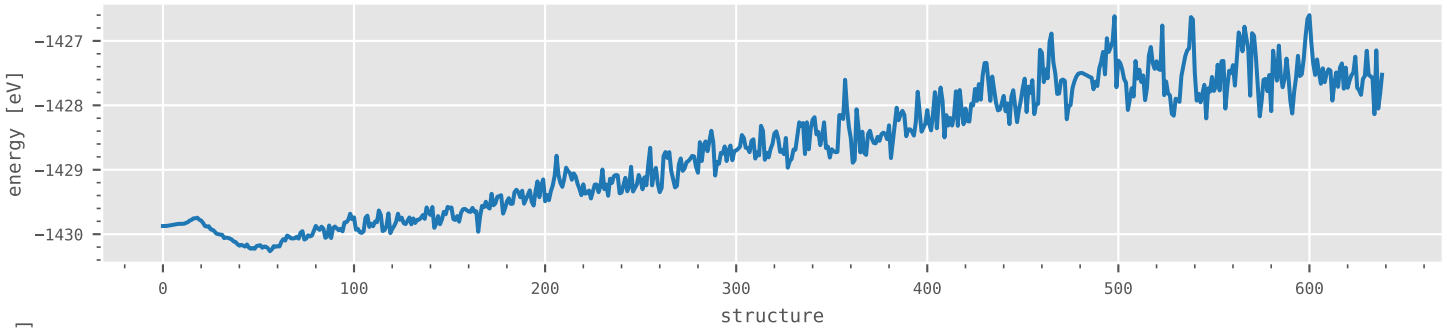
min energy configuration

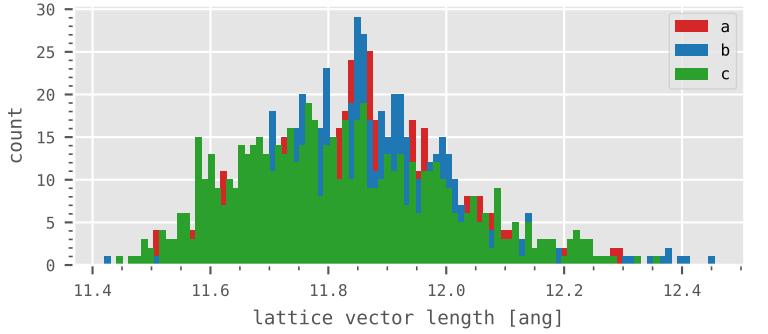


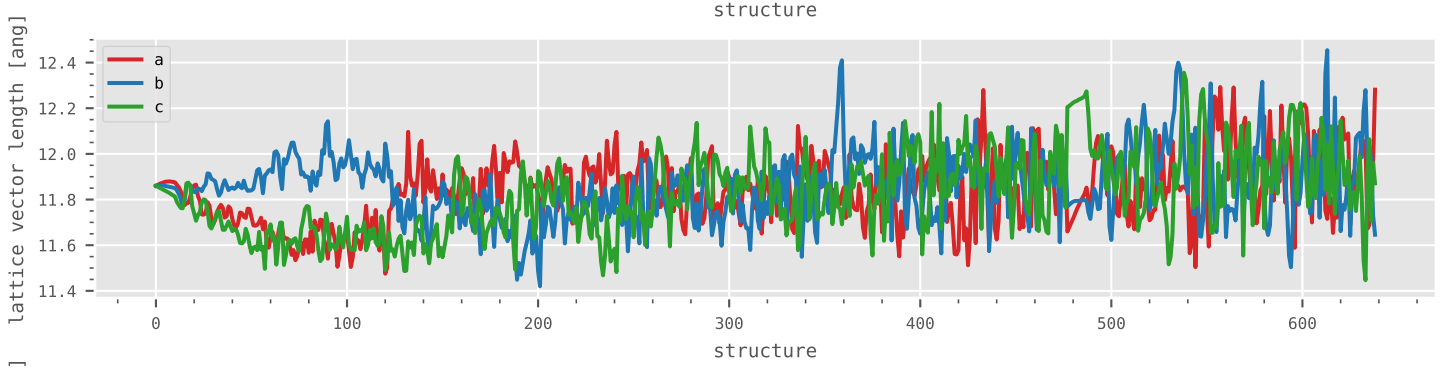
current structure group

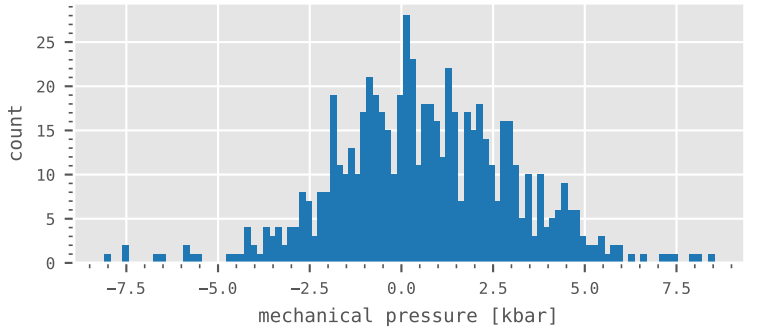
name	CsPbBr3 Cubic MLFF 400 K
structure group	1 (of 1 in file)
structures	639 (of 639 in file)
atoms	Pb (8), Br (24), Cs (8)
	40 total

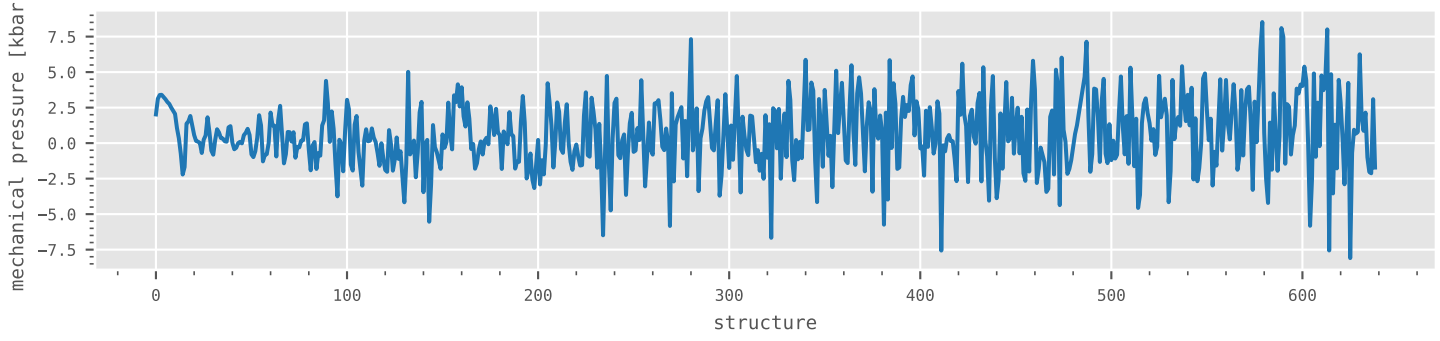




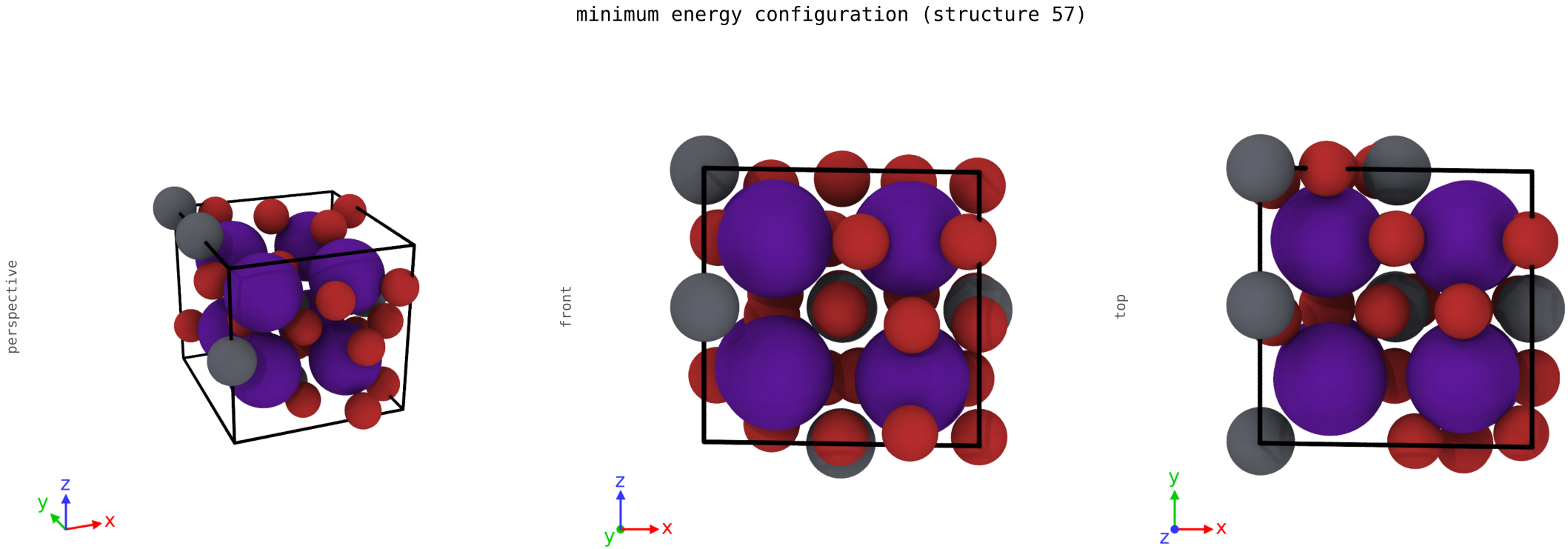




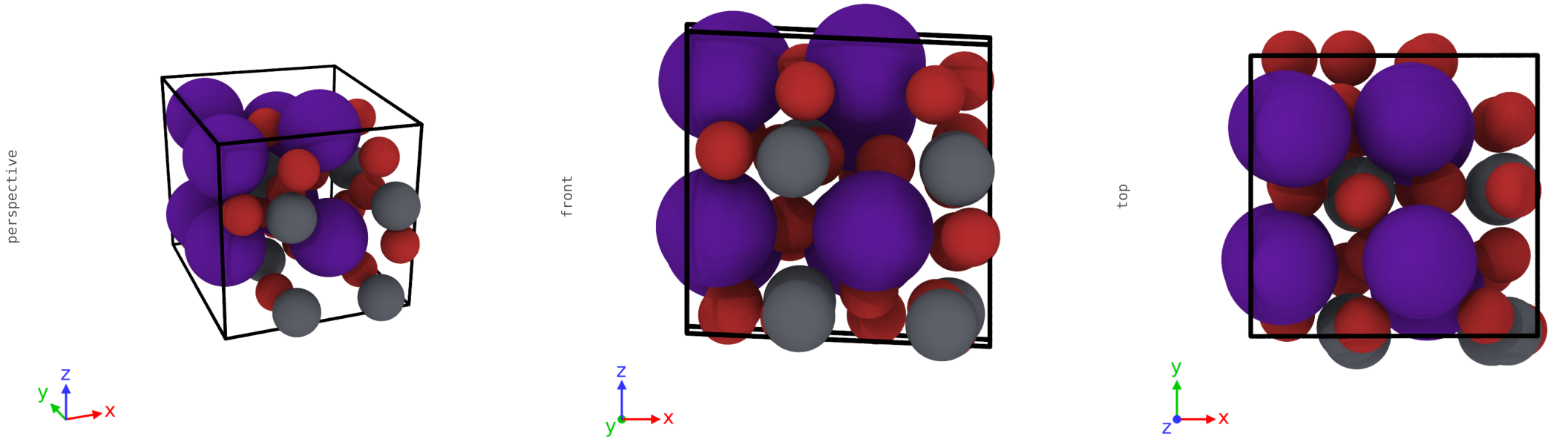


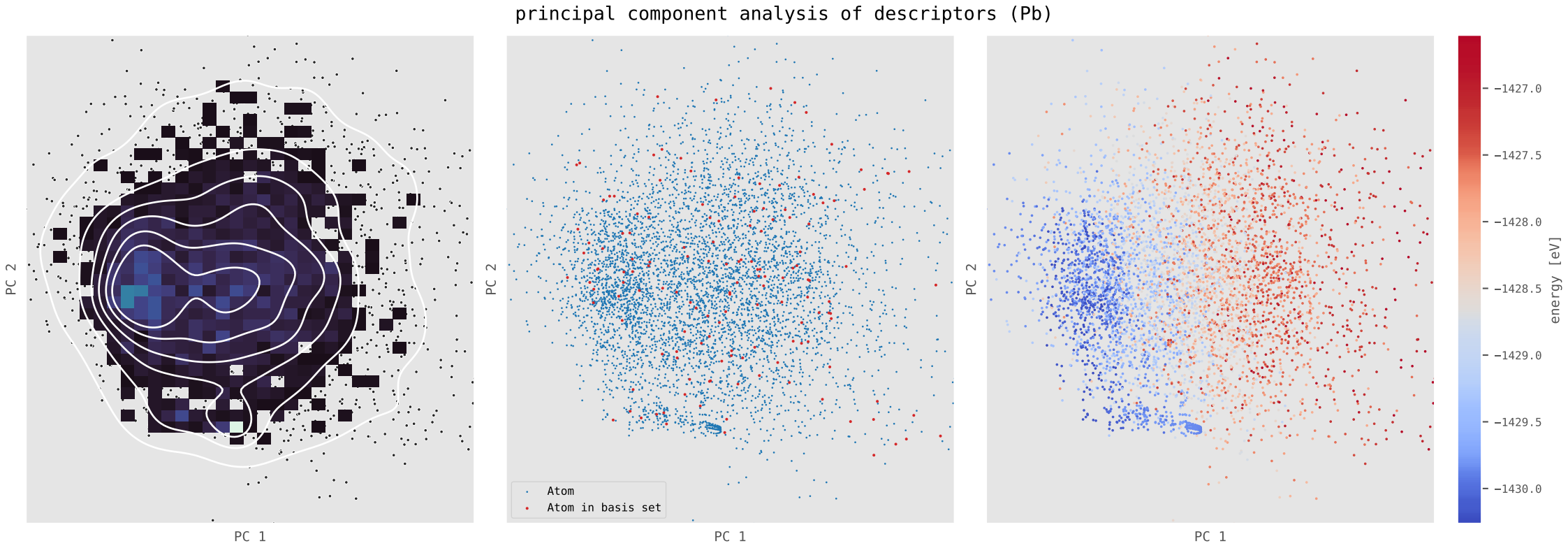


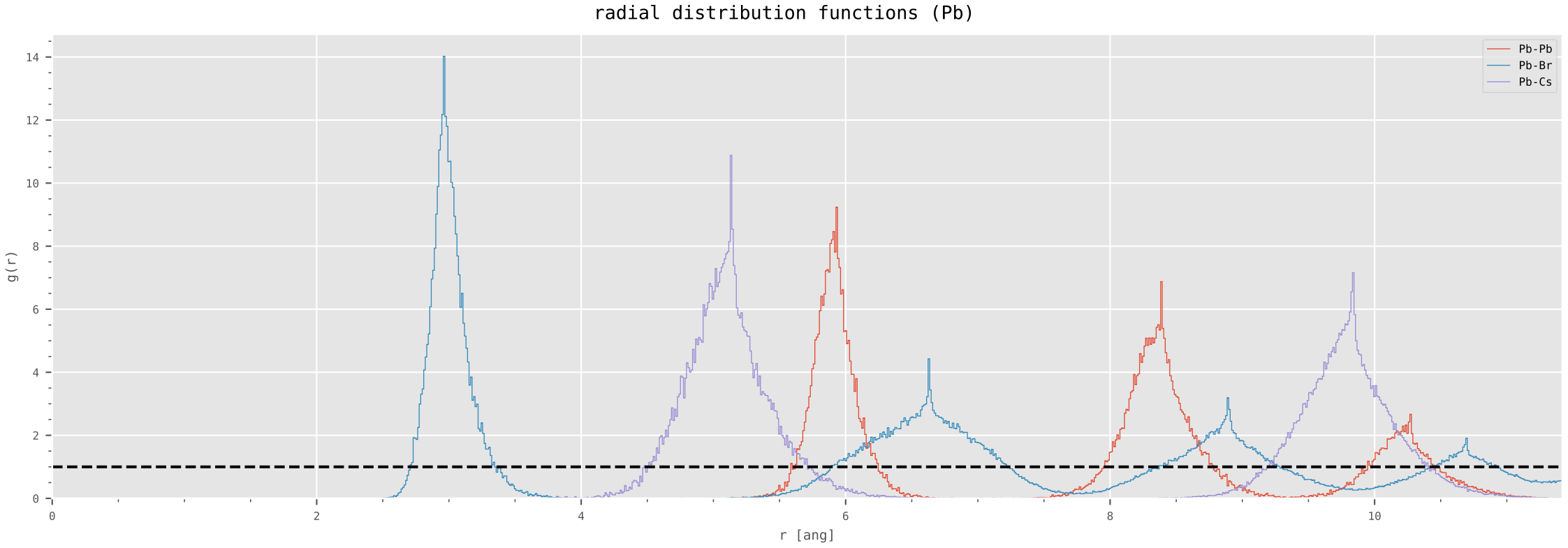
minimum energy configuration (structure 57)



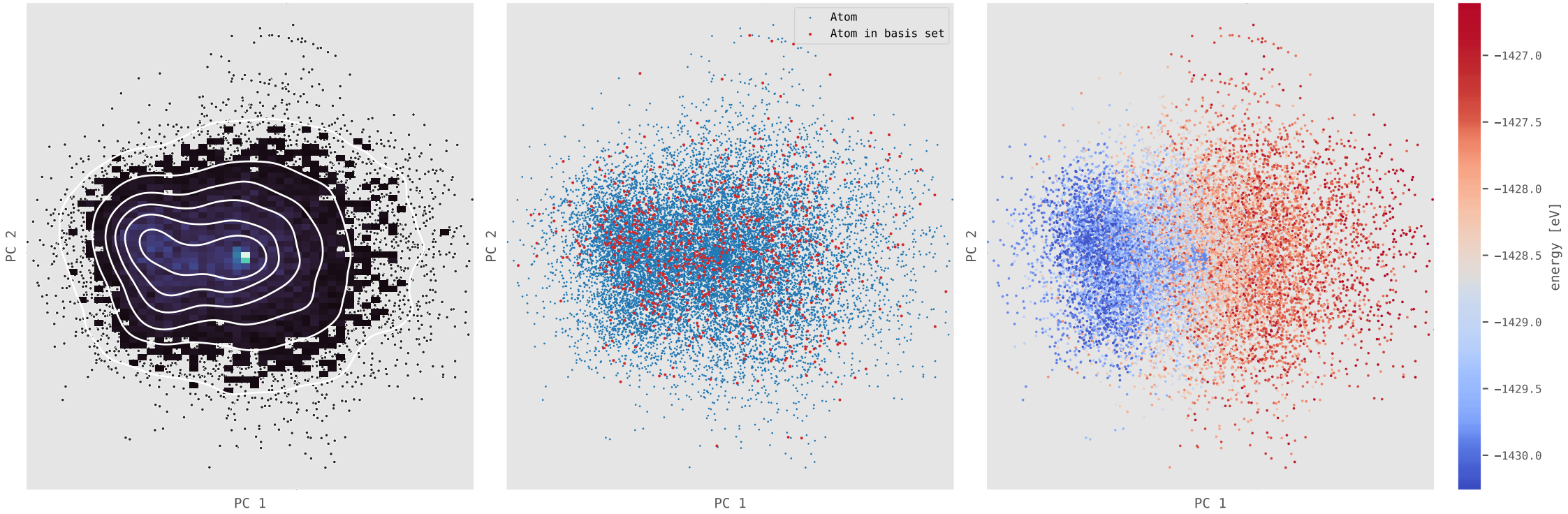
maximum energy configuration (structure 601)



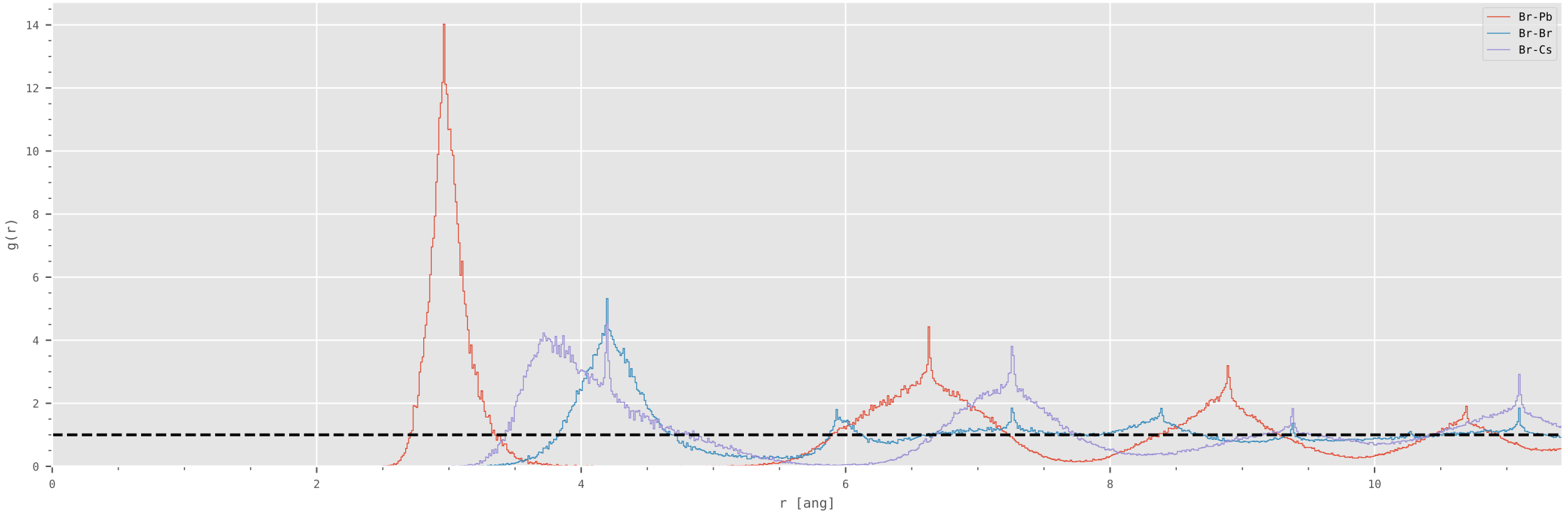

principal component analysis of descriptors (Pb)
PC 2
PC 1
Atom
Atom in basis set
energy [eV]
−1427.0
−1427.5
−1428.0
−1428.5
−1429.0
−1429.5
−1430.0

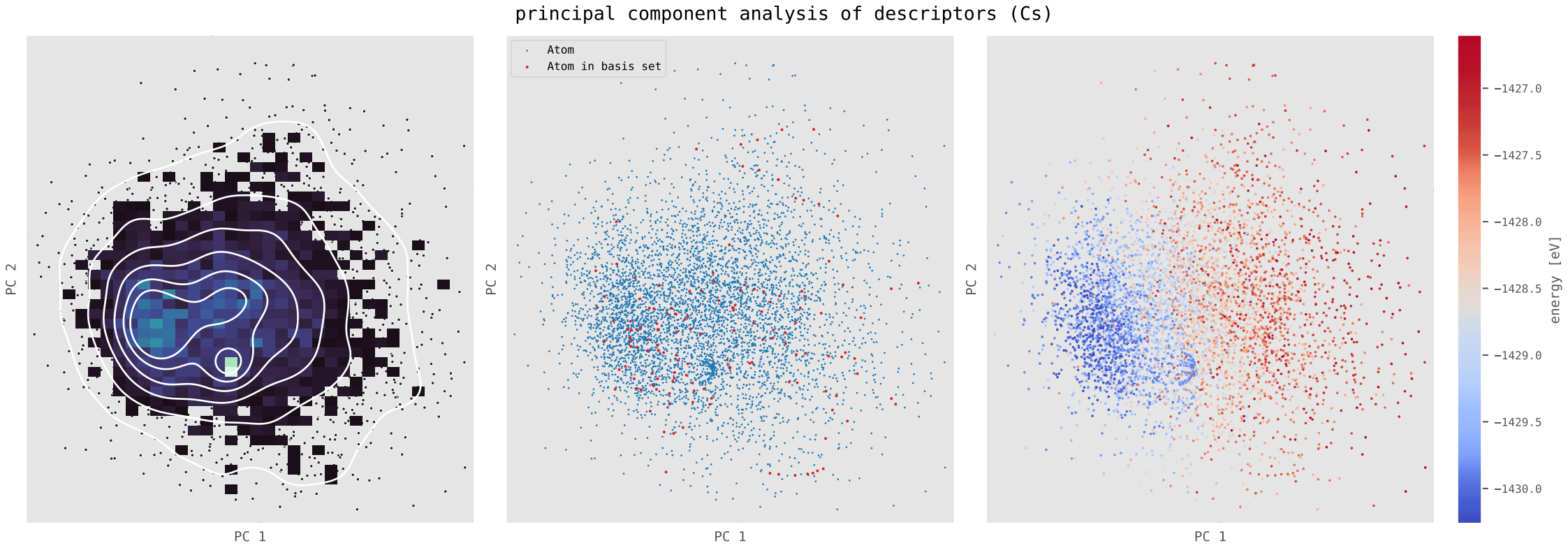

radial distribution functions (Pb)
Pb-Pb
Pb-Br
Pb-Cs
g(r)
r [ang]

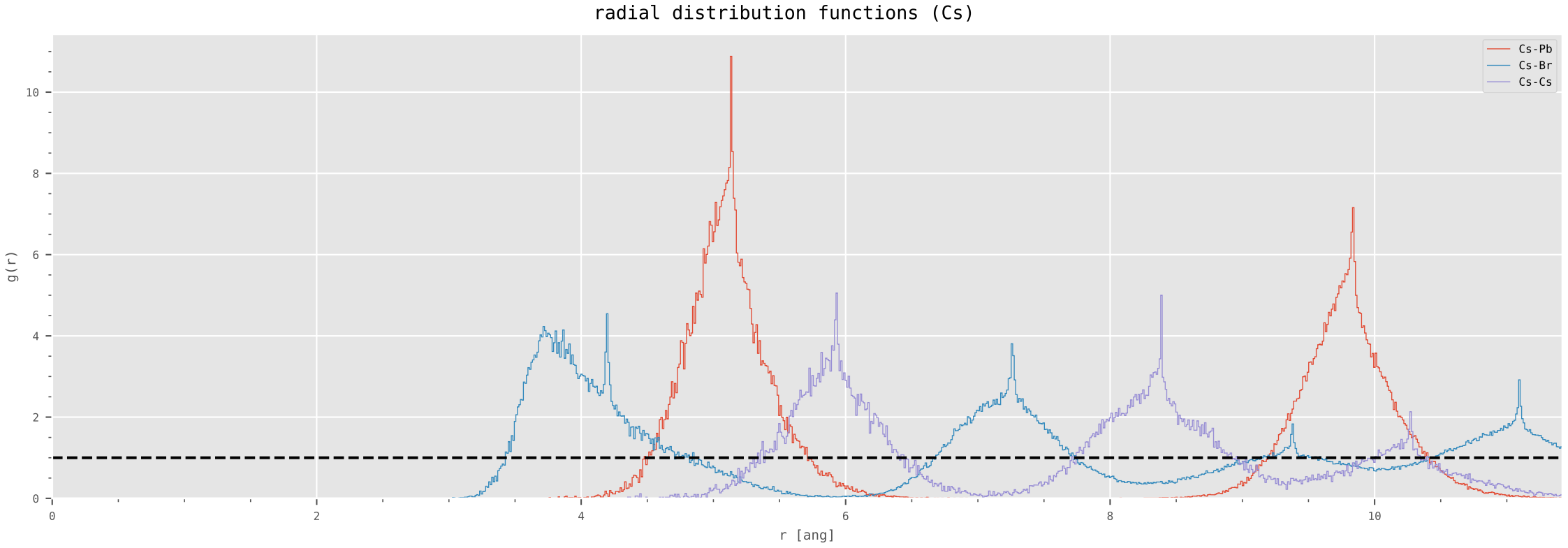
principal component analysis of descriptors (Br)



radial distribution functions (Br)




principal component analysis of descriptors (Cs)
Atom
Atom in basis set
PC 1
PC 2
energy [eV]
−1427.0
−1427.5
−1428.0
−1428.5
−1429.0
−1429.5
−1430.0


radial distribution functions (Cs)
Cs-Pb
Cs-Br
Cs-Cs
g(r)
r [ang]
0
2
4
6
8
10