

[1/1] ML_AB_lightmass (CsPbBr3)

file

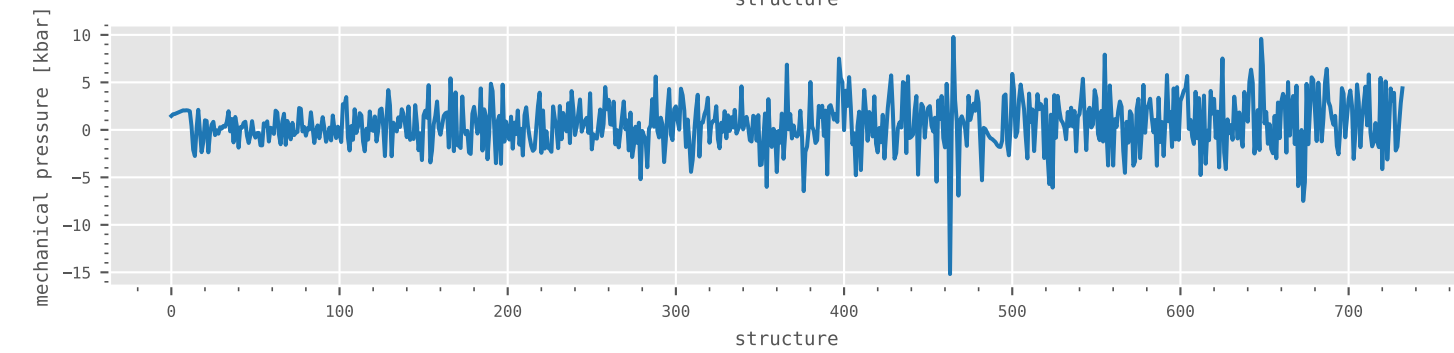
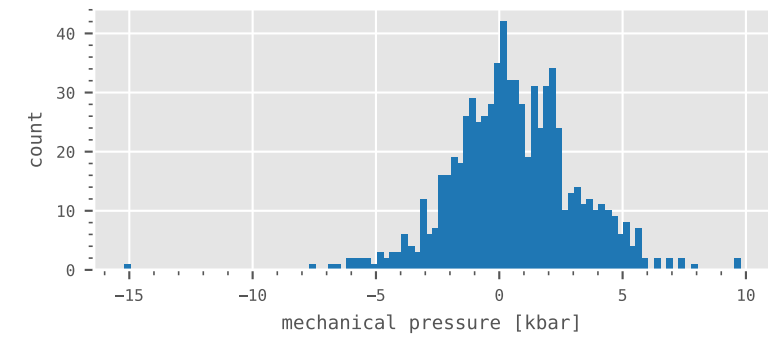
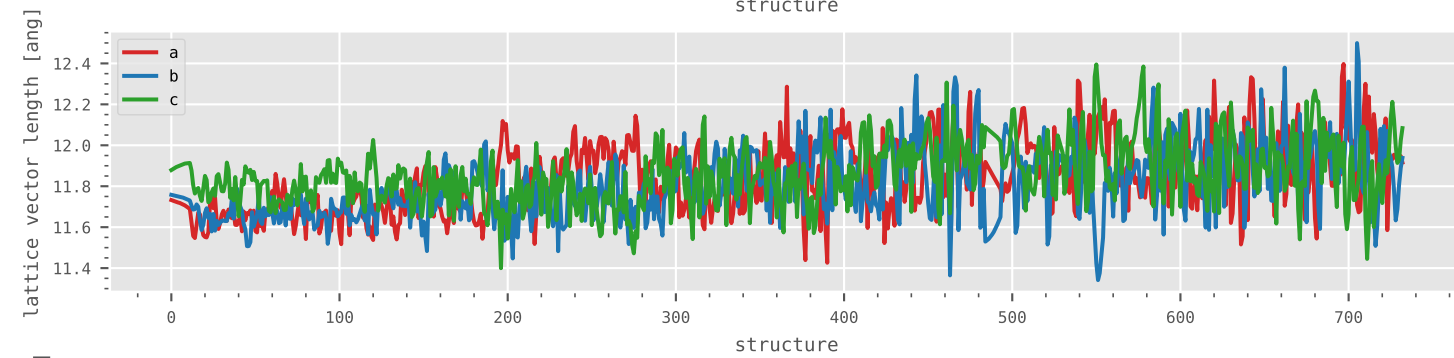
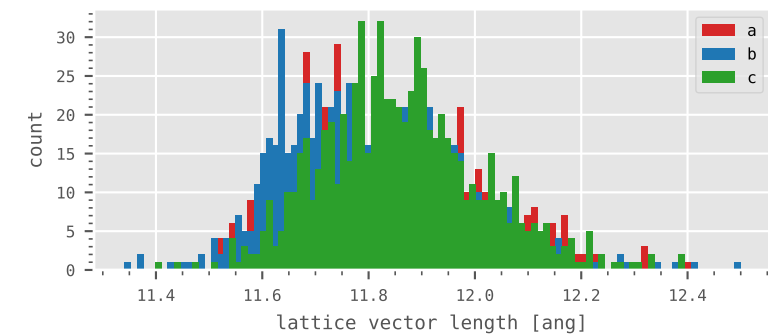
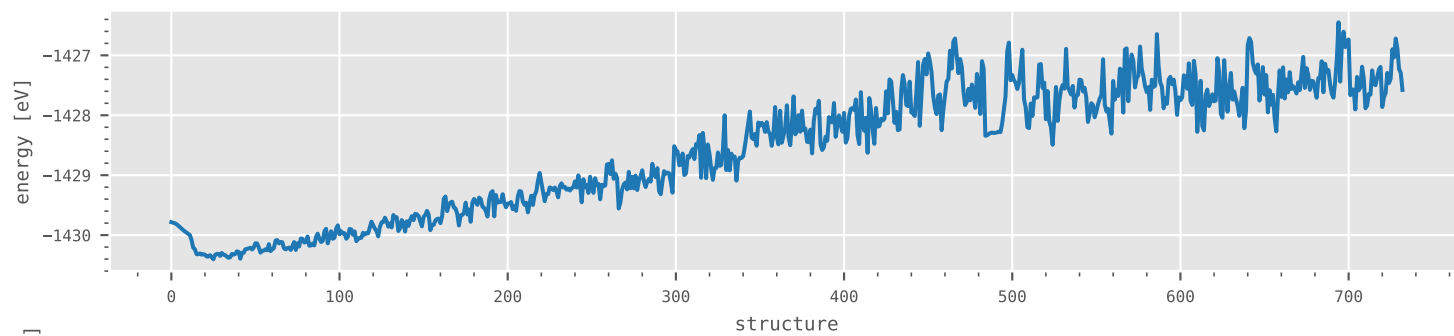
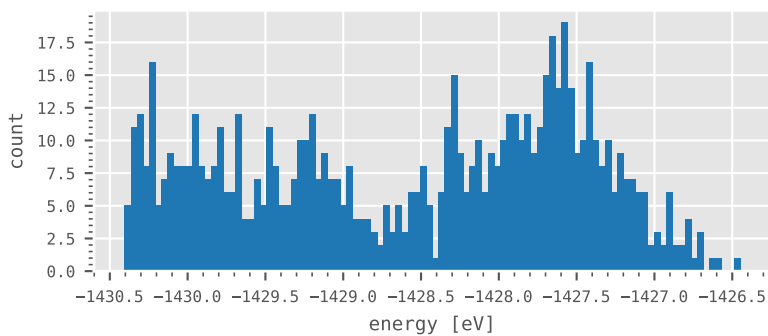
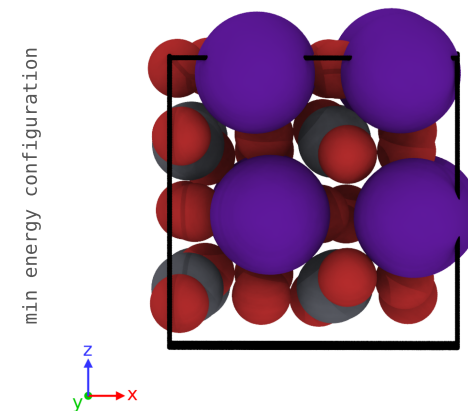
name	ML_AB_lightmass
structure groups	1
total structures	733

overview

energy	-1428.6 ± 1.06	eV
volume	1658.4 ± 41.22	ang ³
lattice vector a	11.8 ± 0.17	ang
lattice vector b	11.8 ± 0.17	ang
lattice vector c	11.9 ± 0.15	ang
non-periodic radius	5.7 (min. for group)	ang

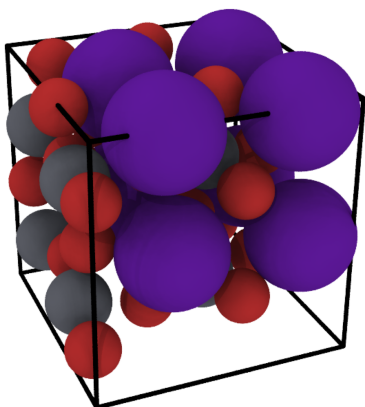
current structure group

name	CsPbBr3
structure group	1 (of 1 in file)
structures	733 (of 733 in file)
atoms	Pb (8), Br (24), Cs (8)
	40 total

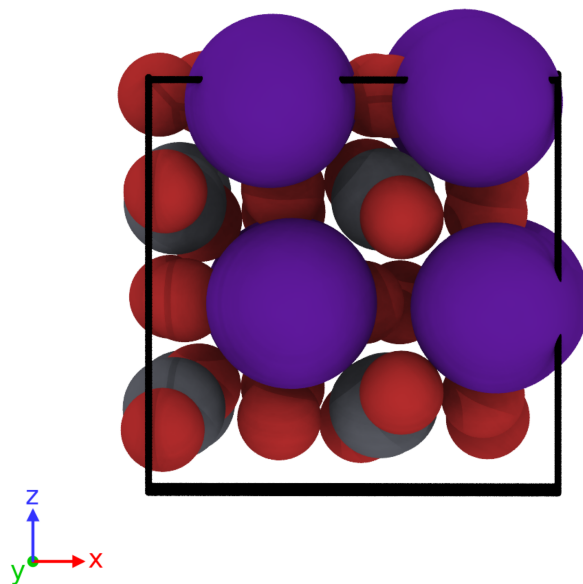


minimum energy configuration (structure 26)

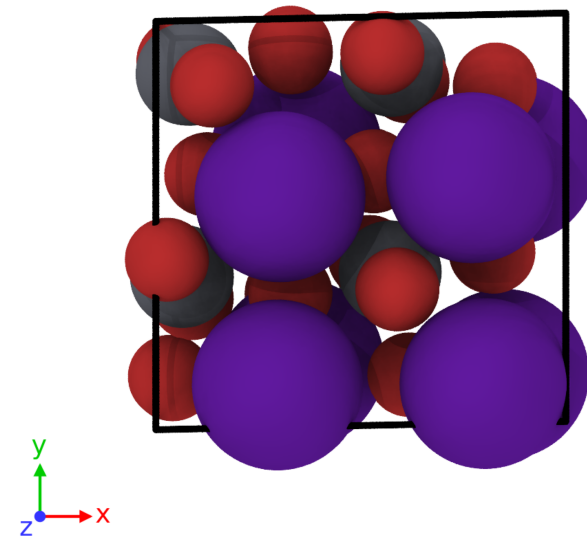
perspective



front

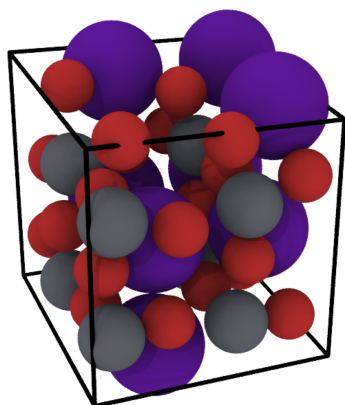


top

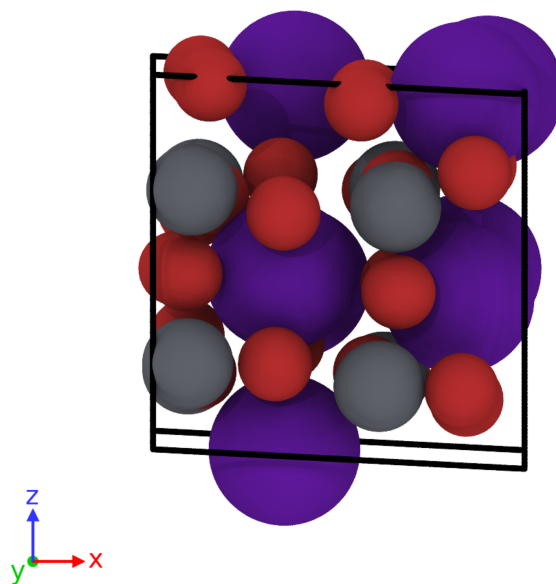


maximum energy configuration (structure 695)

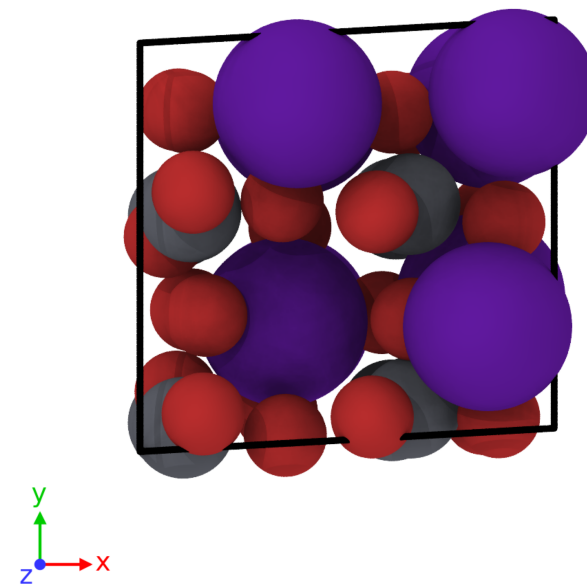
perspective



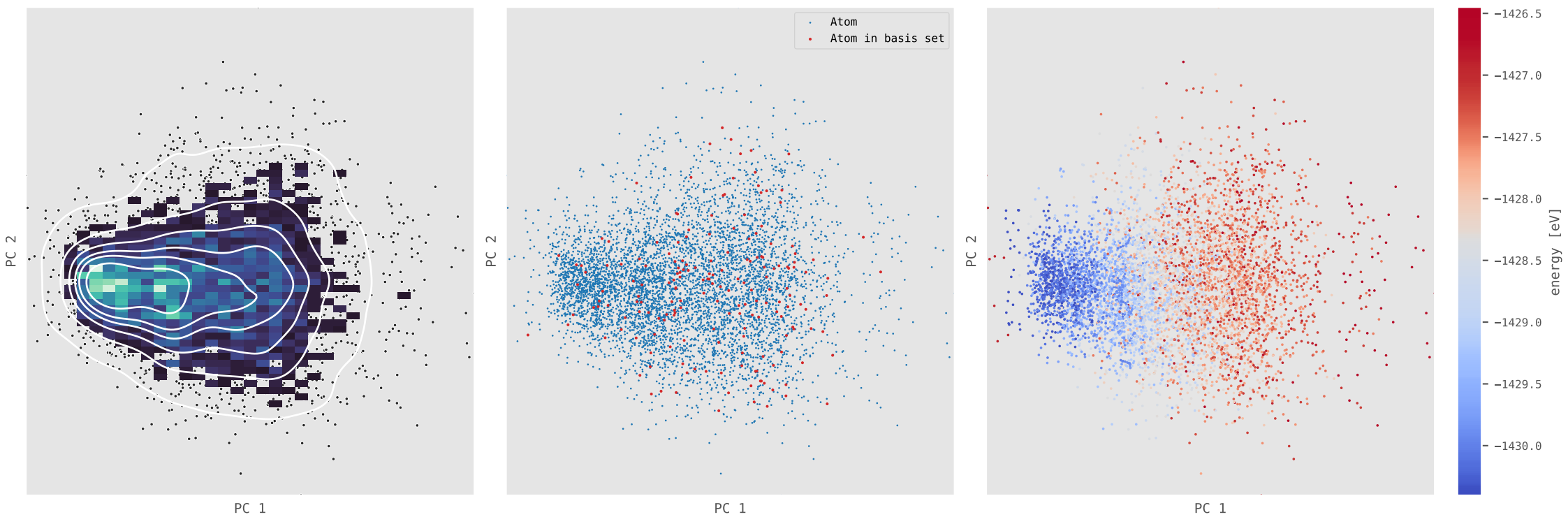
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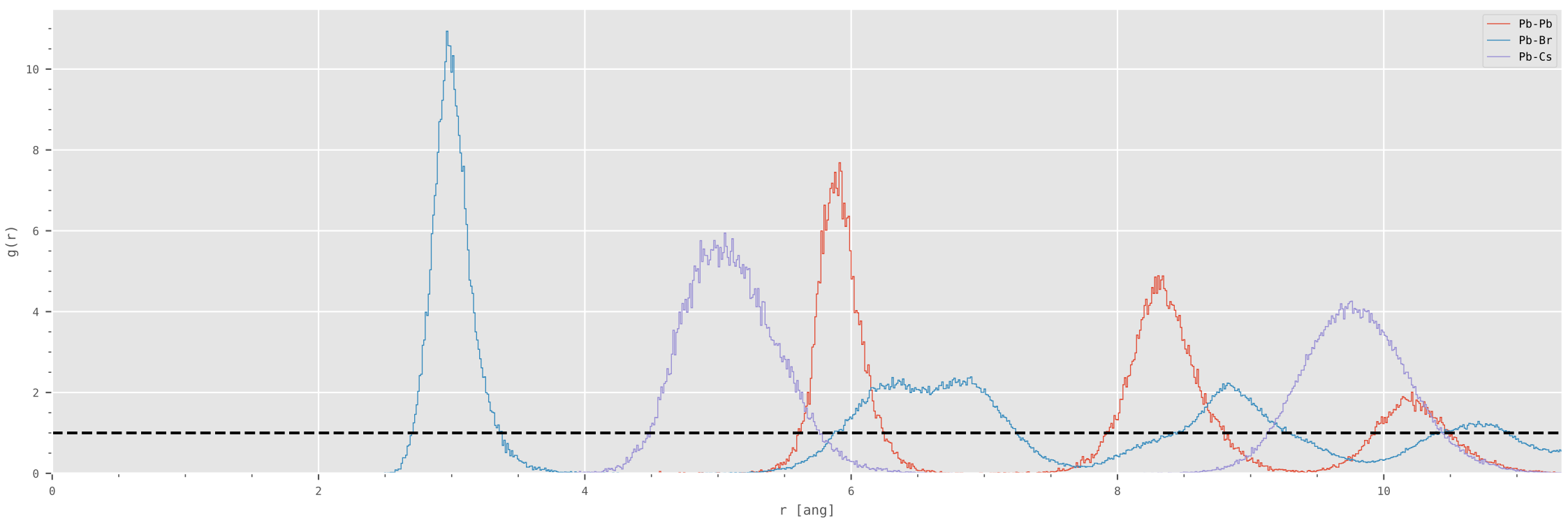
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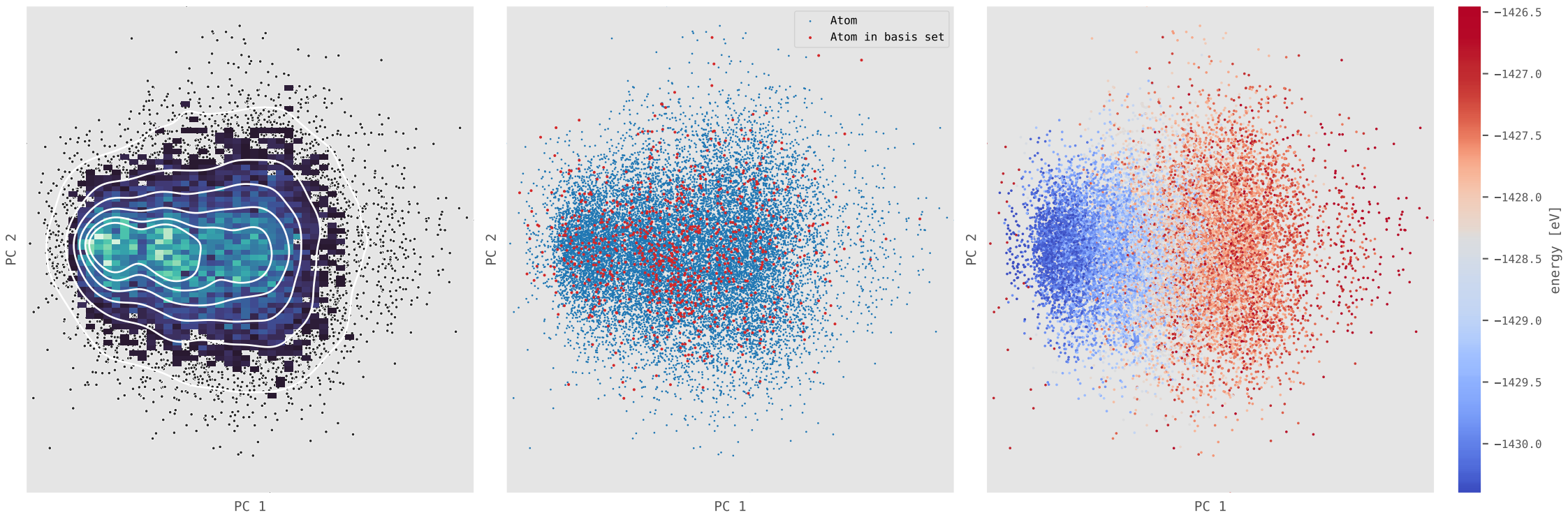
principal component analysis of descriptors (Pb)



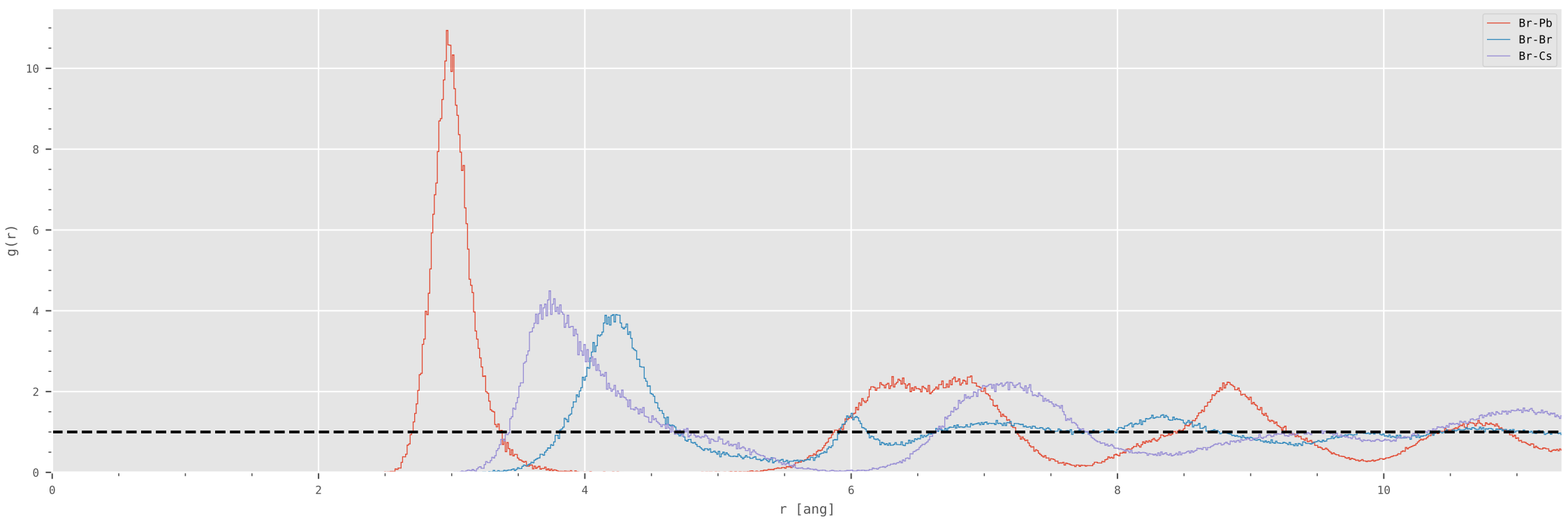
radial distribution functions (Pb)



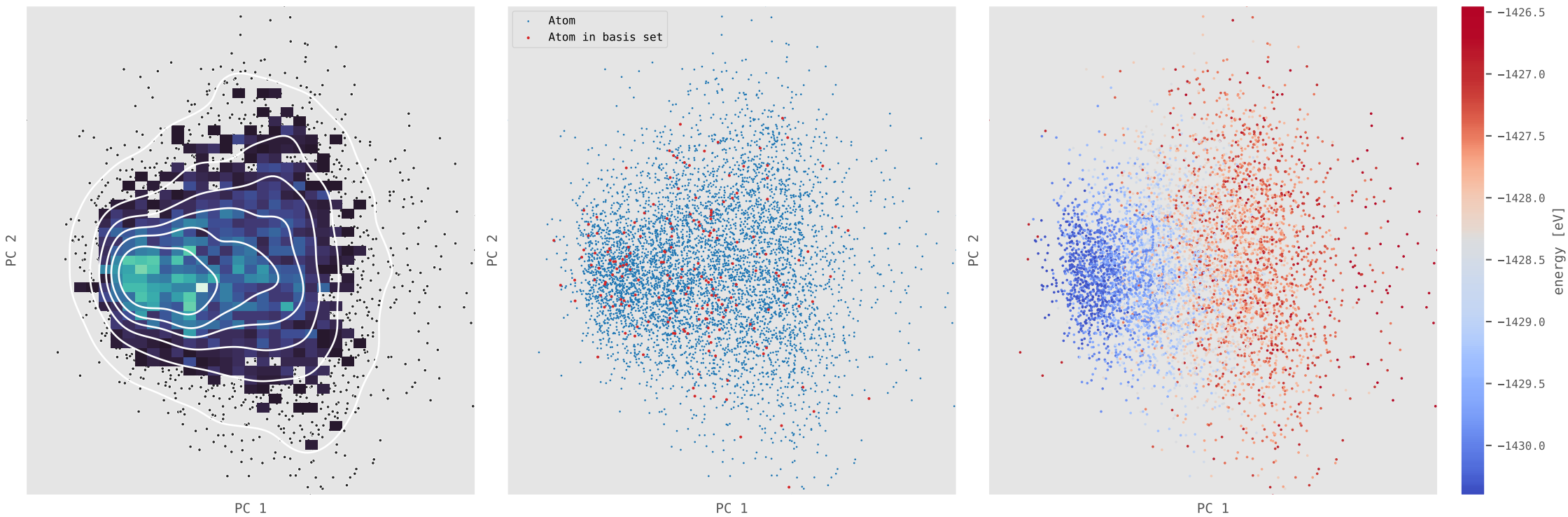
principal component analysis of descriptors (Br)



radial distribution functions (Br)



principal component analysis of descriptors (Cs)



radial distribution functions (Cs)

