

[1/1] ML_AB_BiO_small (Bi2)

file

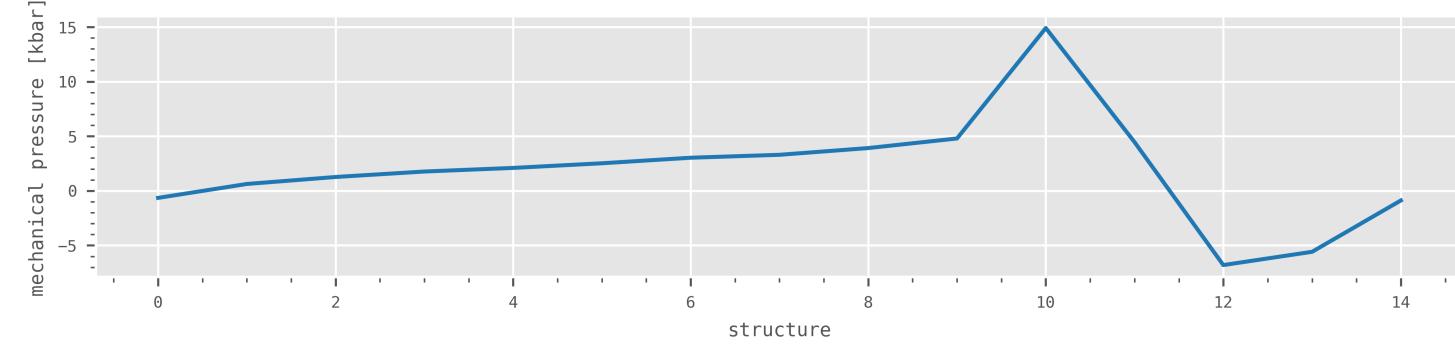
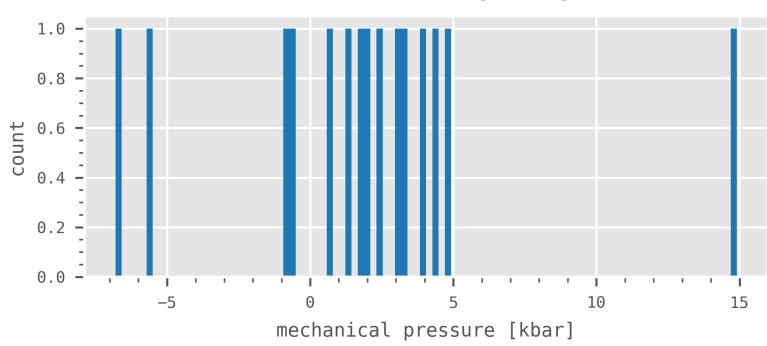
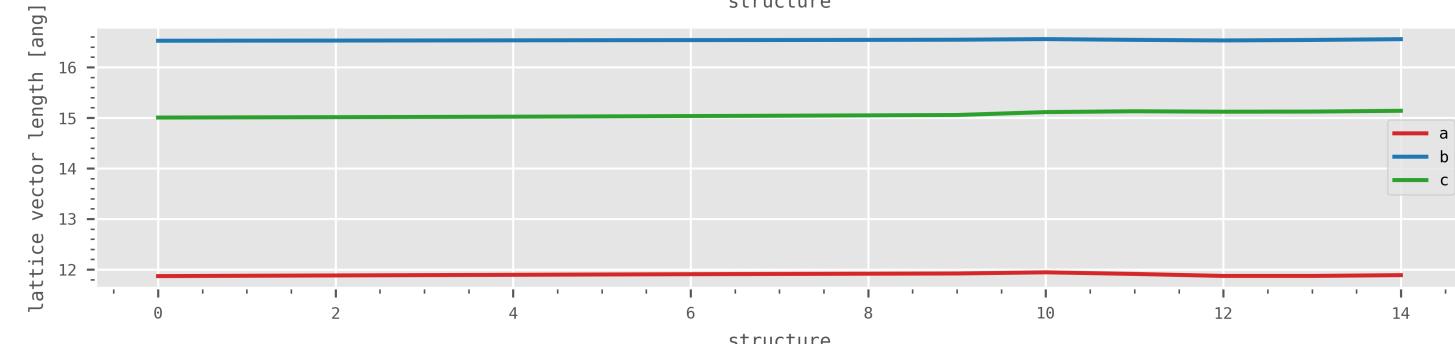
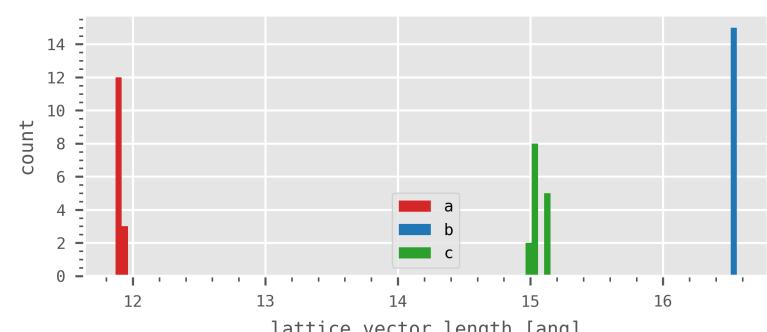
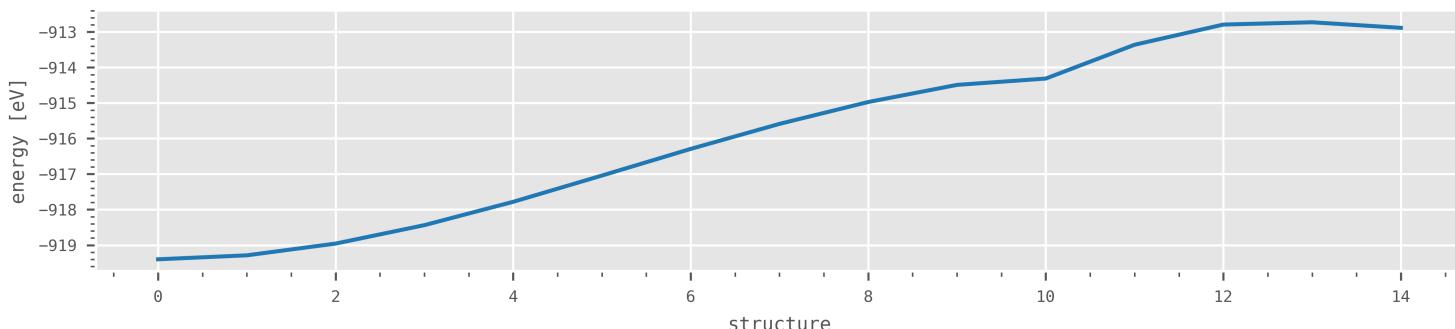
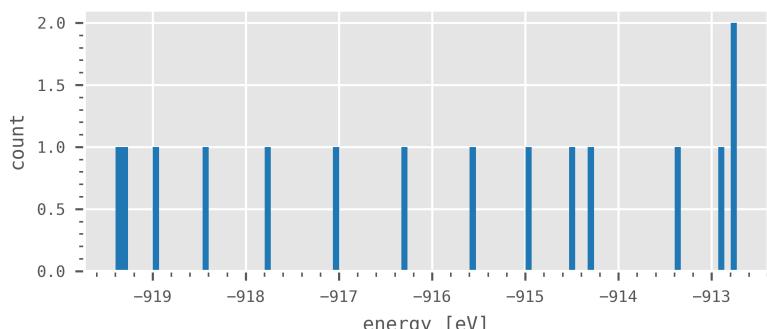
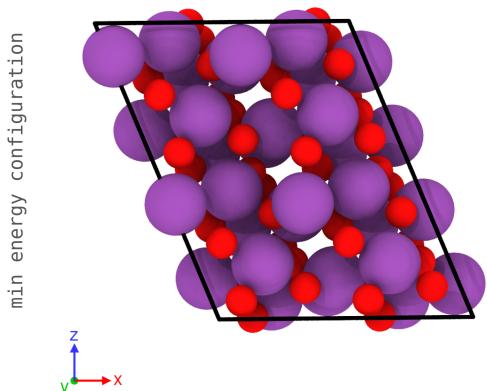
name ML_AB_BiO_small
 structure groups 1
 total structures 15

overview

energy	-915.9 ± 2.47	eV
volume	2963.3 ± 13.51	ang^3
lattice vector a	11.9 ± 0.02	ang
lattice vector b	16.5 ± 0.01	ang
lattice vector c	15.1 ± 0.05	ang
non-periodic radius	5.9 (min. for group)	ang

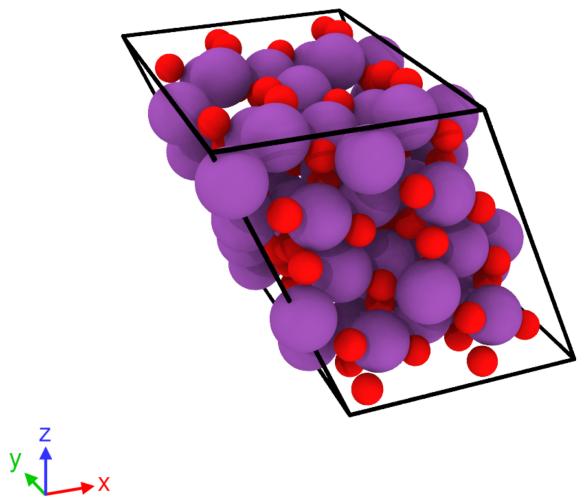
current structure group

name Bi2
 structure group 1 (of 1 in file)
 structures 15 (of 15 in file)
 atoms Bi (64), O (96)
 160 total

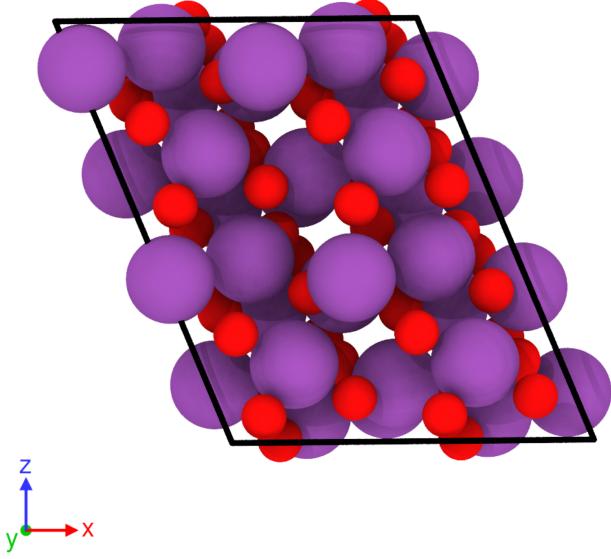


minimum energy configuration (structure 1)

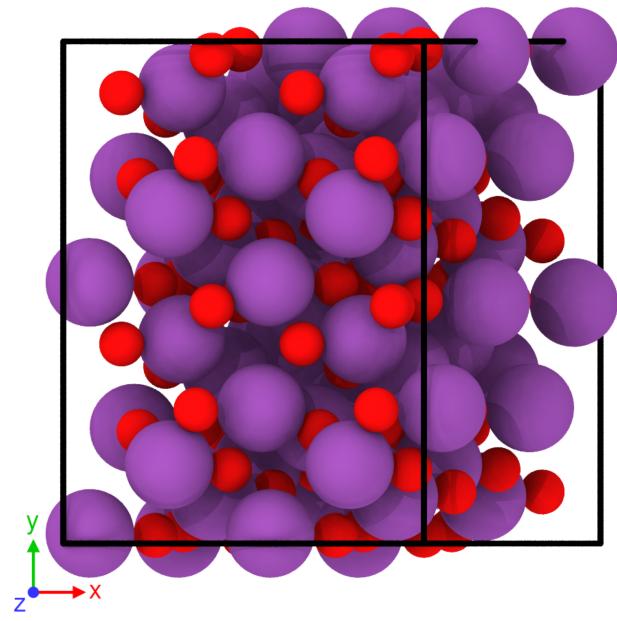
perspective



front

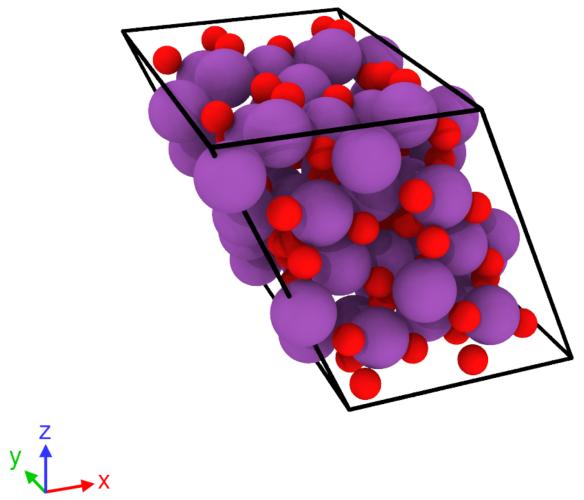


top

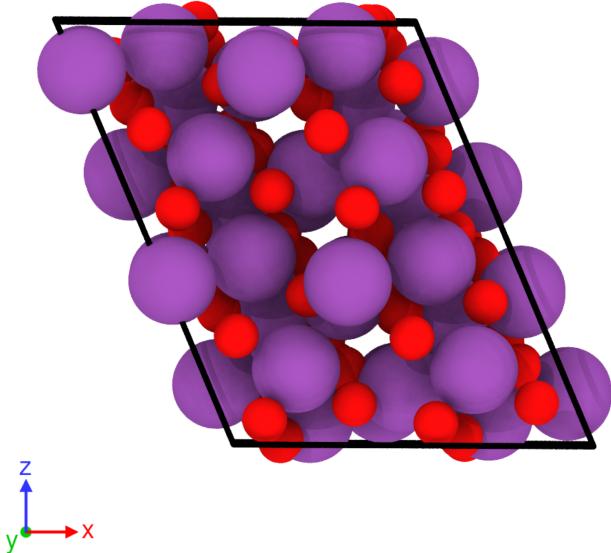


maximum energy configuration (structure 14)

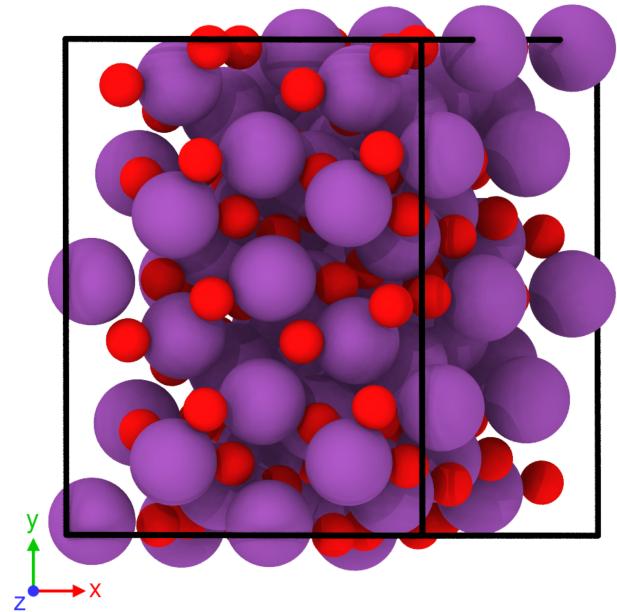
perspective



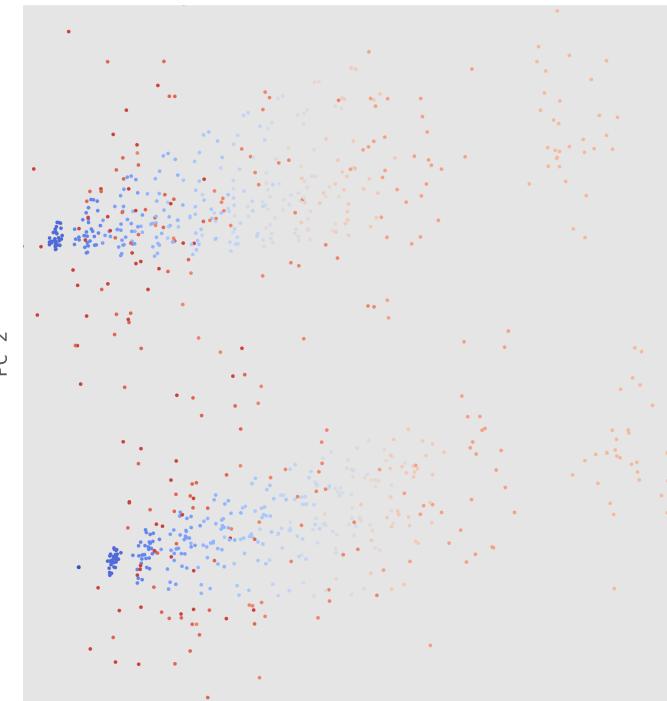
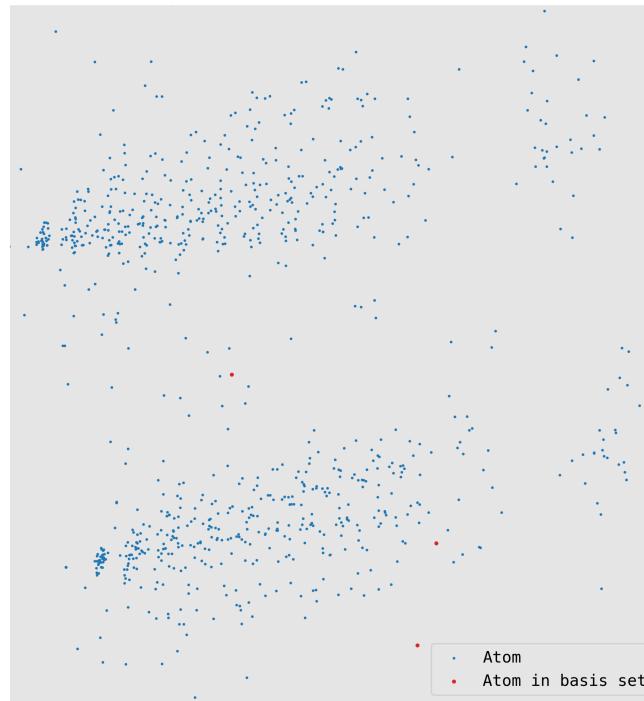
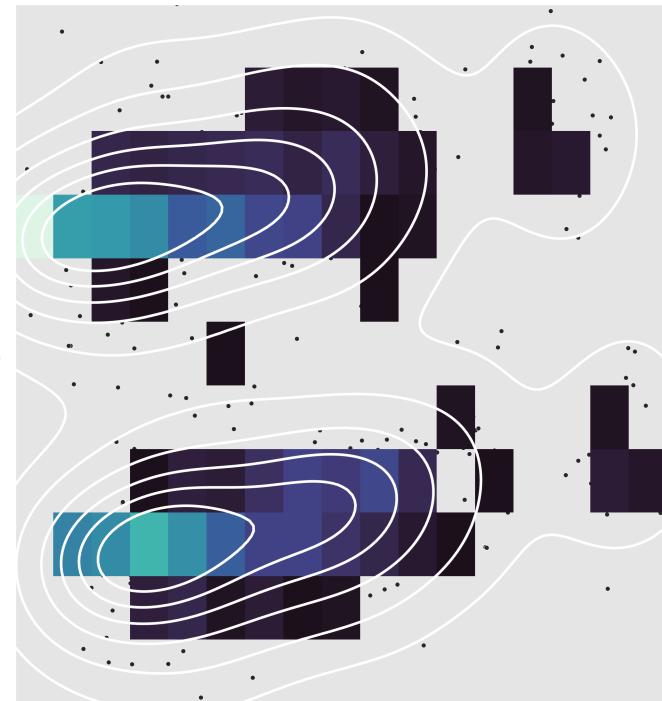
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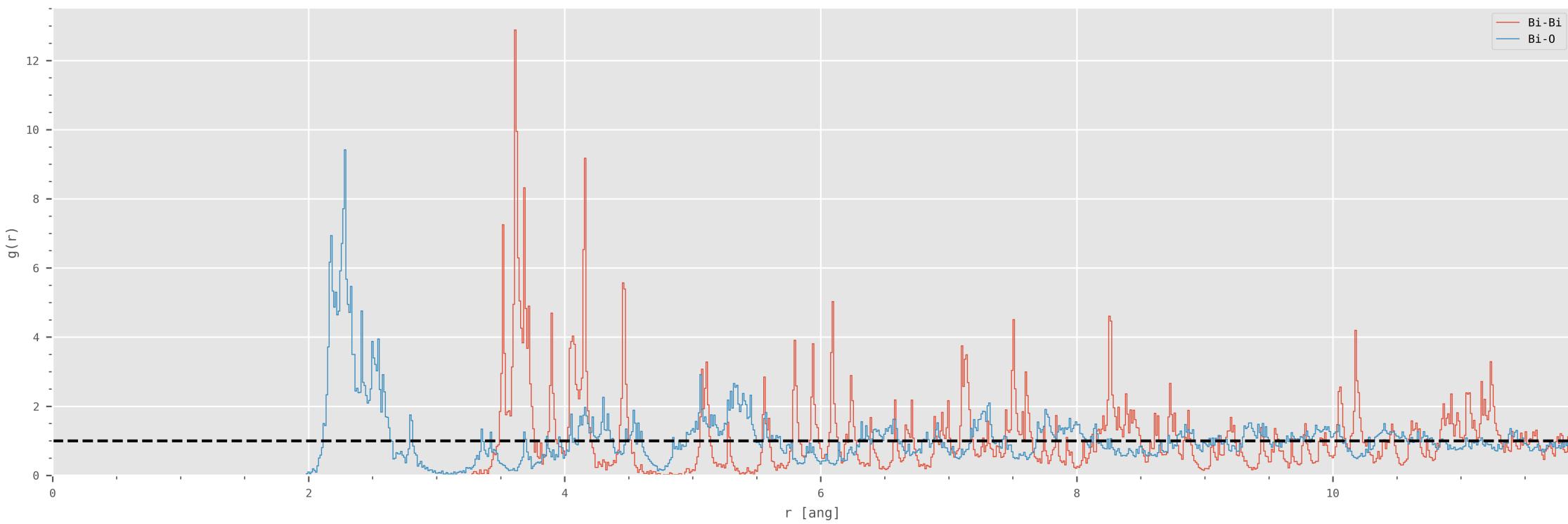
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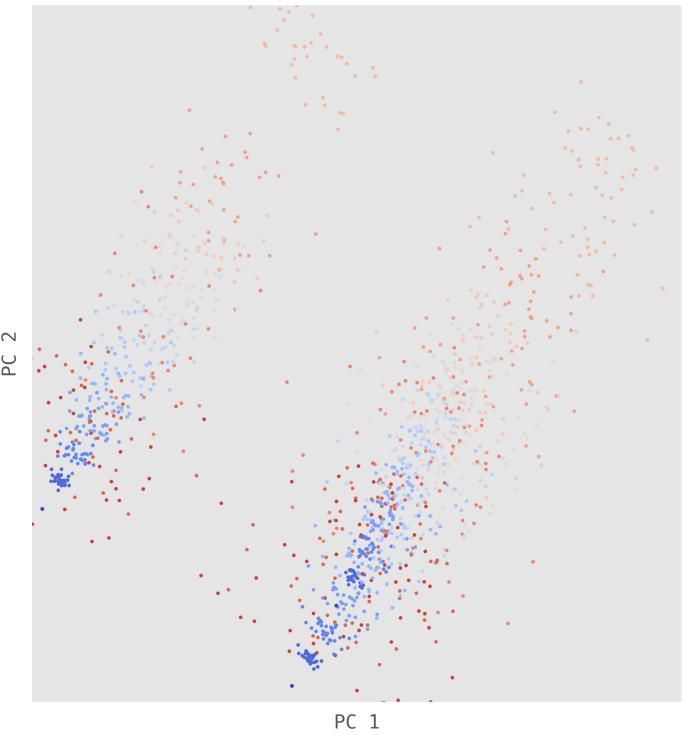
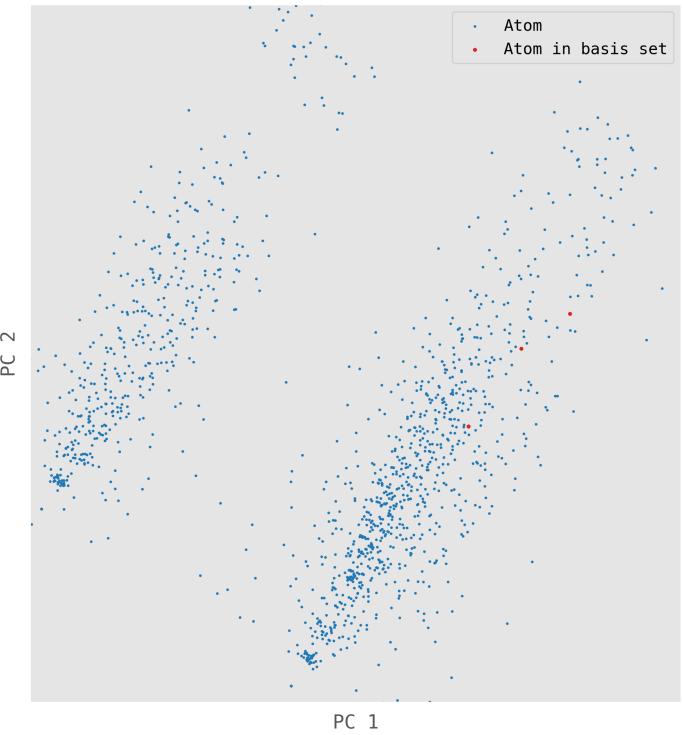
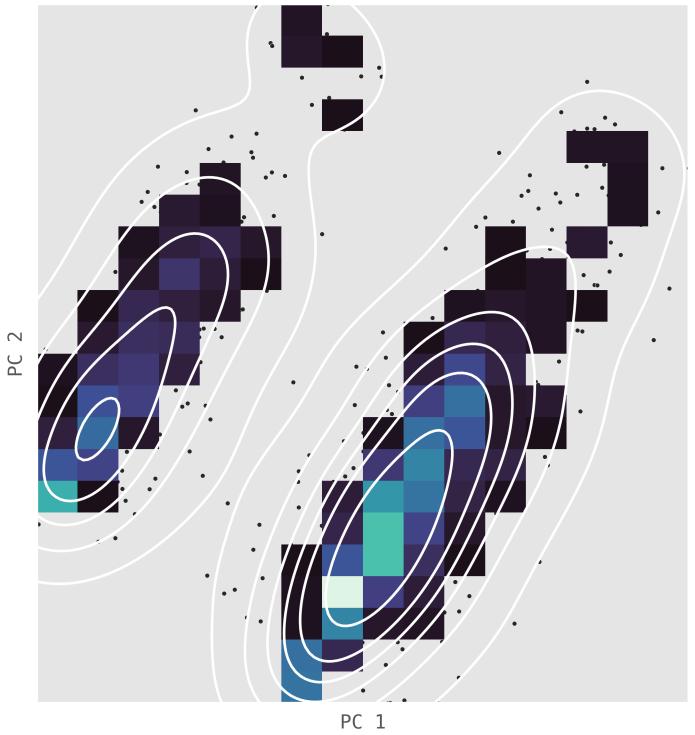
principal component analysis of descriptors (Bi)



radial distribution functions (Bi)



principal component analysis of descriptors (0)



radial distribution functions (0)

