Figure Outline for Computational Perovskite Alloys Dataset

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Outline

DFT simulation premise I

Perovskite structure summary

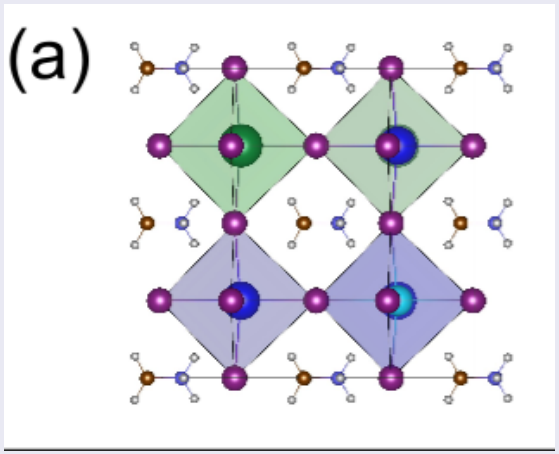

Figure: ABX_3 Cubic Perovskite Structure

Perovskite Chemical Domain

Table: ABX_3 Chemical Domain

A-site	B-site	X-site
MA	Pb	I
FA	Sn	Br
Cs	Ge	Cl
Rb	Ba	
K	Sr	
	Ca	
	Be	
	Mg	
	Si	
	V	
	Cr	
	Mn	
	Fe	
	Ni	
	Zn	

Composition Space Sampling I

construction of simulations

Table: Mix Table

cell construct	trials
2x2x2 Supercell A-site mixed	126
2x2x2 B & X-site mixed	5
2x2x2 Supercell B-site mixed	151
3x3x3 Supercell B-site mixed	5
4x4x4 Supercell B-site mixed	10
Alternative B-site elements	36
2x2x2 Pure	90
2x2x2 X-site mixed	127

Composition Space Sampling II

Sampling in DFT dataset

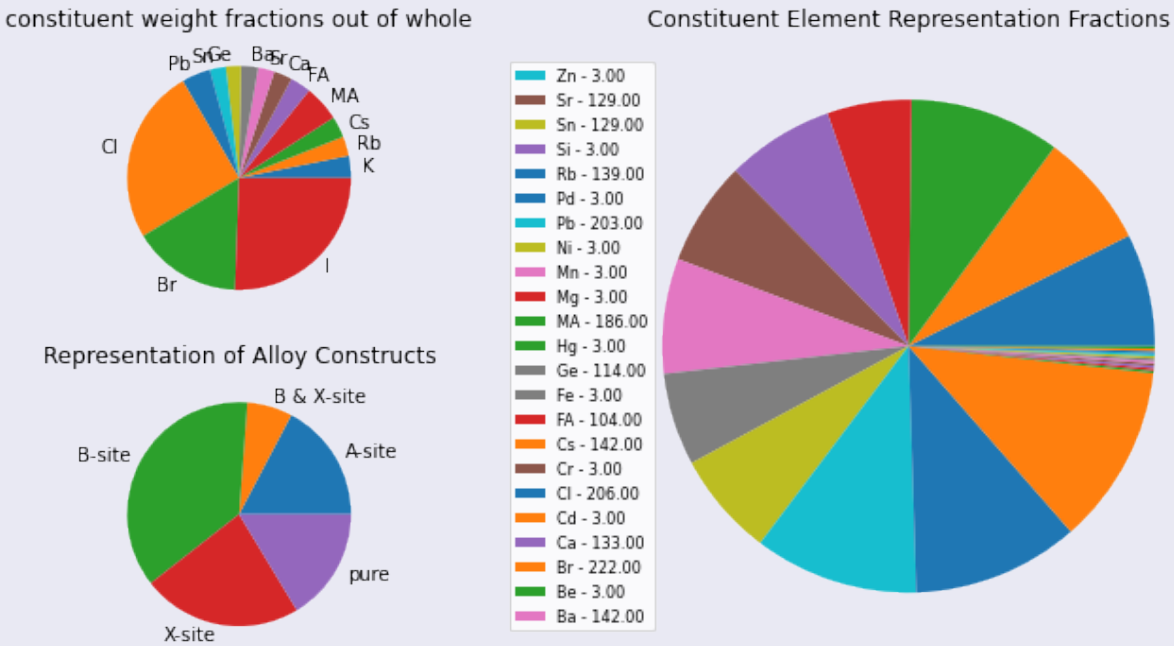

Figure: Species by weight and frequency, and alloy representations in DFT dataset

Composition Space Sampling III

Sampling in experimental dataset

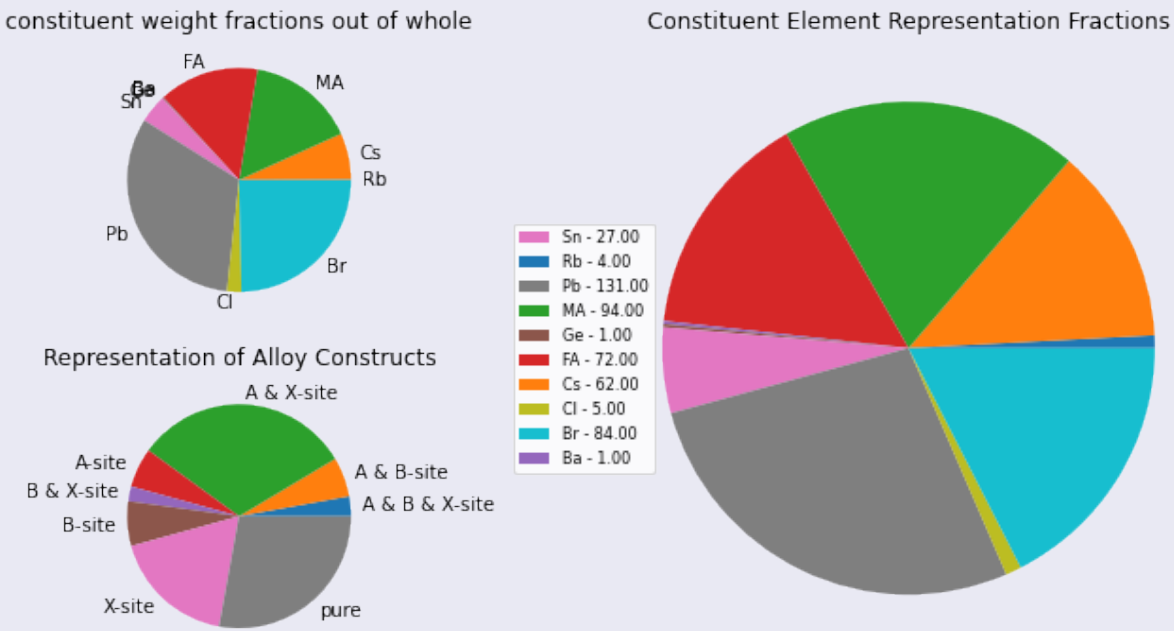

Figure: Species by weight and frequency, and alloy representations in experimental dataset to date

Topology of Composition Space I

PCA projection of Mannodi compositions

PCA projection of Experimental compositions

Computational vs Experimental I

Band Gaps

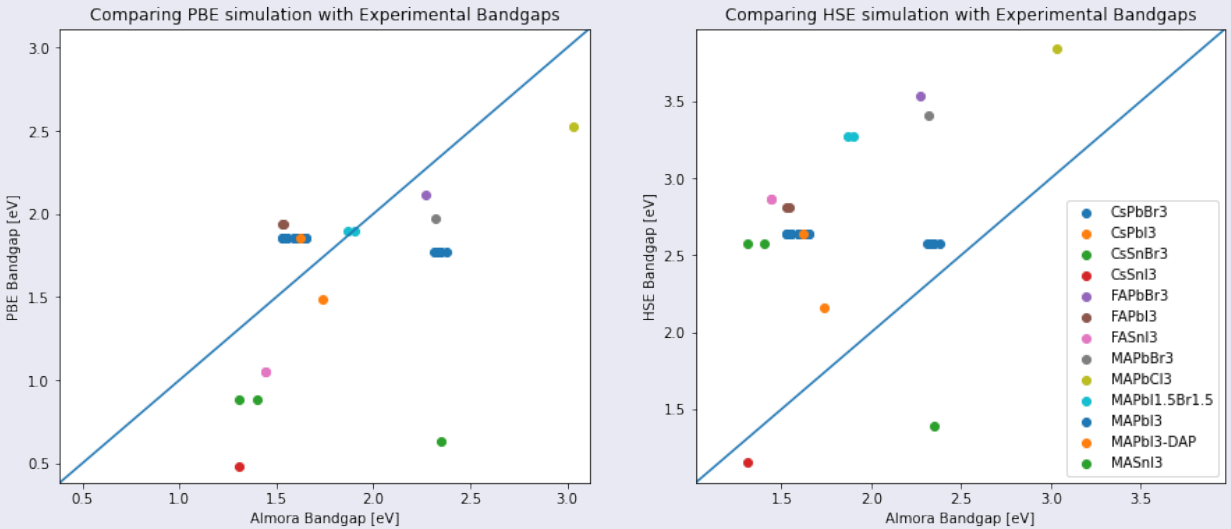

Figure: HSE and PBE bandgaps vs experimental measures show clearly computation methods need improvement