MATSUS-2026 Spring

High-throughput and Data-Driven Search for Stable Optoelectronic $AMSe_3$ Materials

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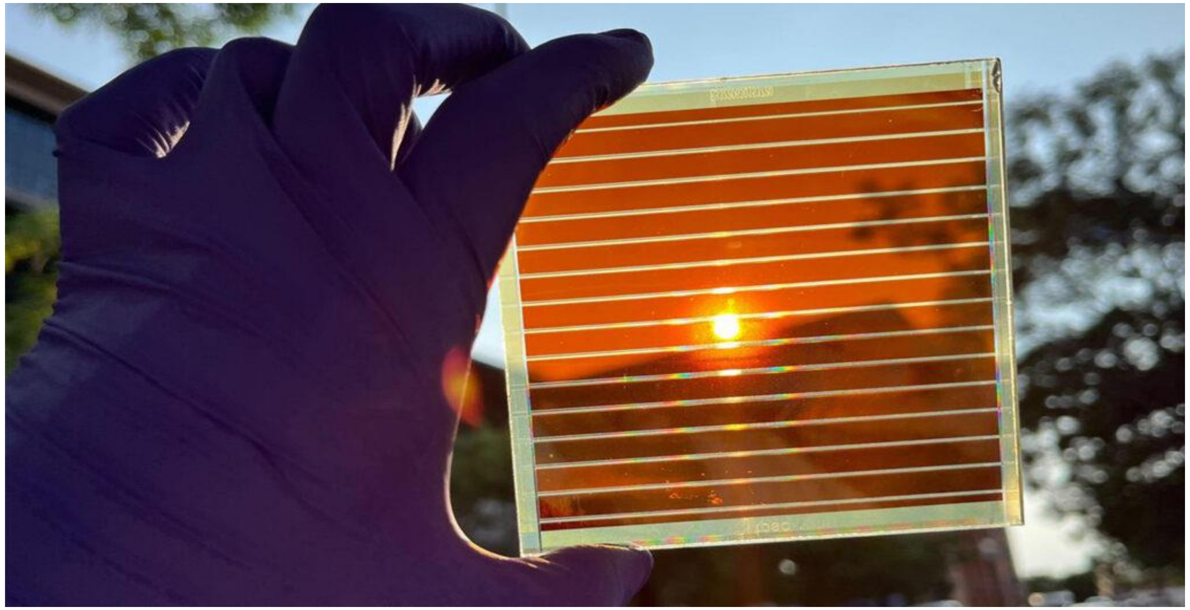
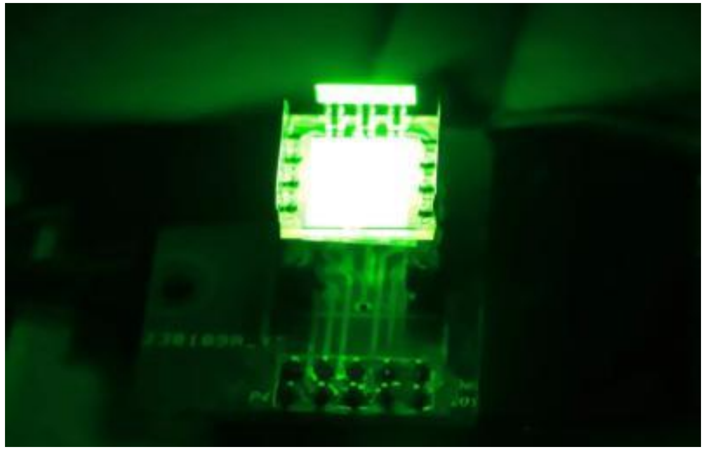
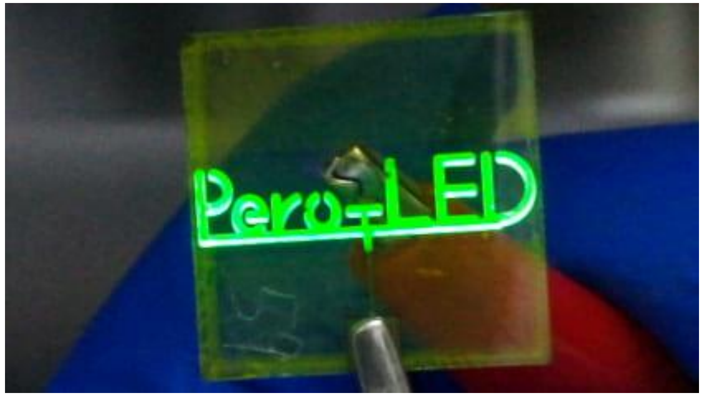
25th March 2026

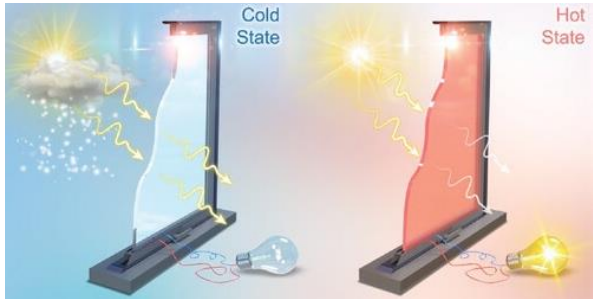
Introduction

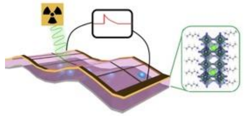
Energy production and efficient usage– An important Quest today











[1] IIT Delhi
[2] Zhejiang University
[3] Nanyang Technological University
[4] SciTech Daily (https://scitechdaily.com/new-discovery-advances-flexible-solar-cells-a-step-closer-to-reality/)
[5] Maysun Solar

Importance of alternatives?

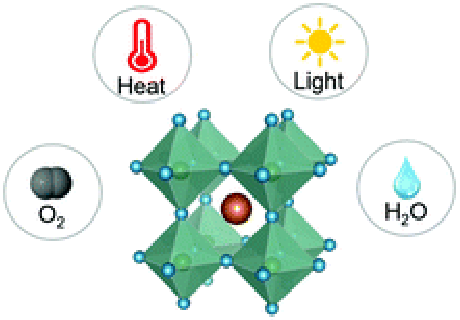
Why explore alternative optoelectronic materials?

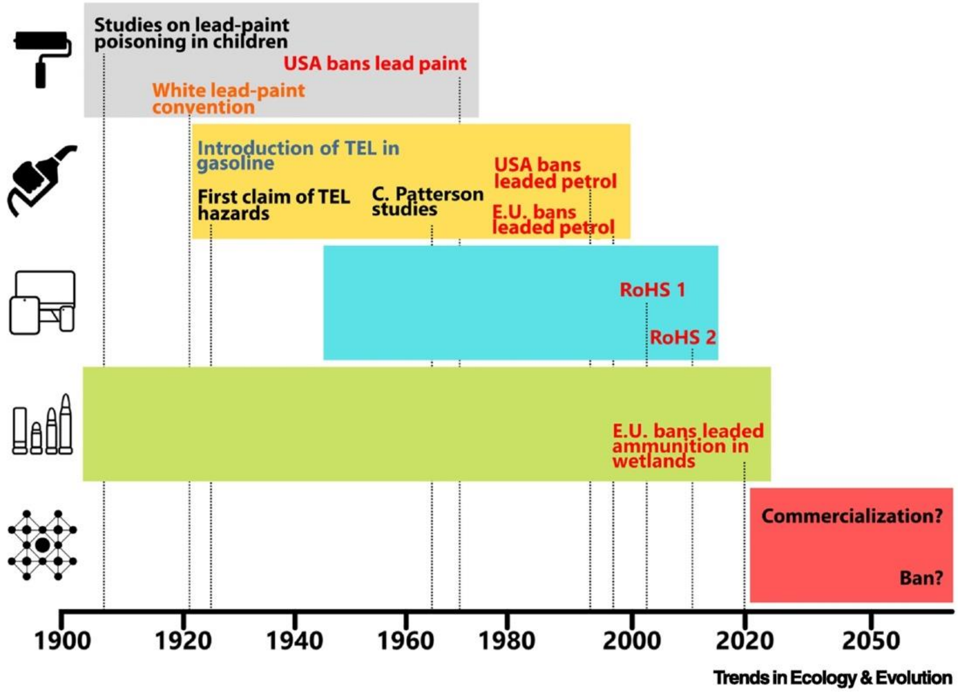
Issues with Silicon:

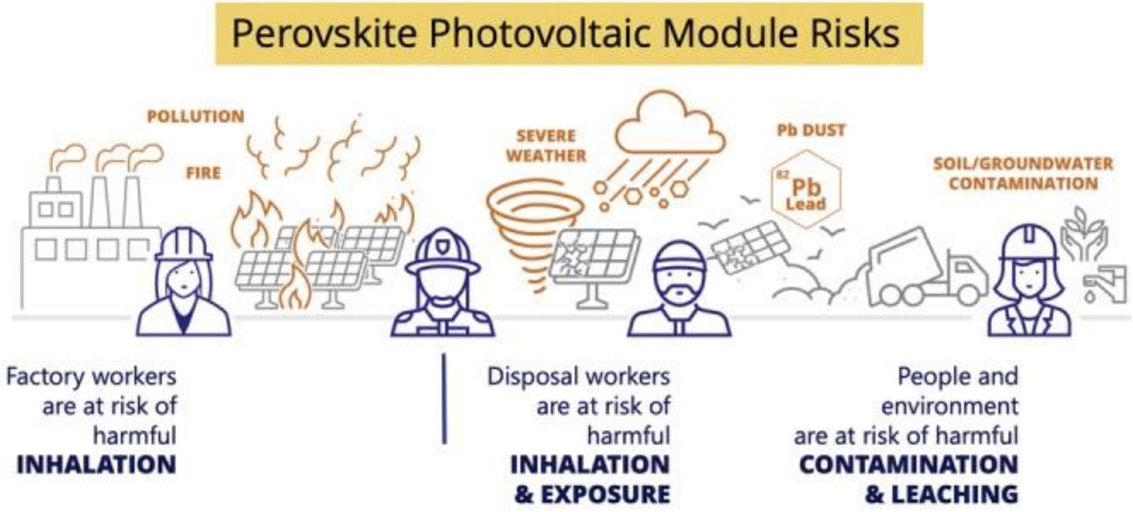
1. Limited efficiency
2. Space constraints to install Si-based PV
3. Rigidity
4. High Fabrication cost

Issues with Pb-based perovskites:

1. Toxicity
2. Stability
3. Device Efficiency







[1] C. Ponti, G. Nasti, D. Di Girolamo, I. Cantone, F. A. Alharthi, A. Abate, *Trends in Ecology & Evolution* 2022, *37*, 281.
[2] C. E. Torrence, C. S. Libby, W. Nie, J. S. Stein, *iScience* 2022, *26*, 105807.

Methodology

Density Functional Theory

Structural optimization & stability analysis
Static electronic properties

Ab initio Molecular Dynamics (AIMD)

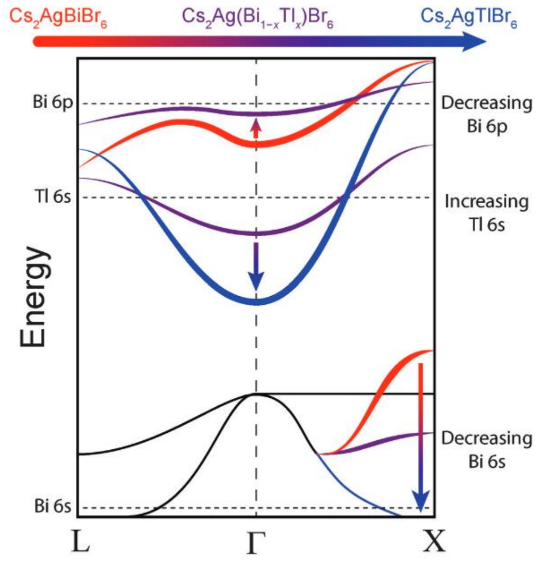
Real-time structural dynamics, dynamic interaction

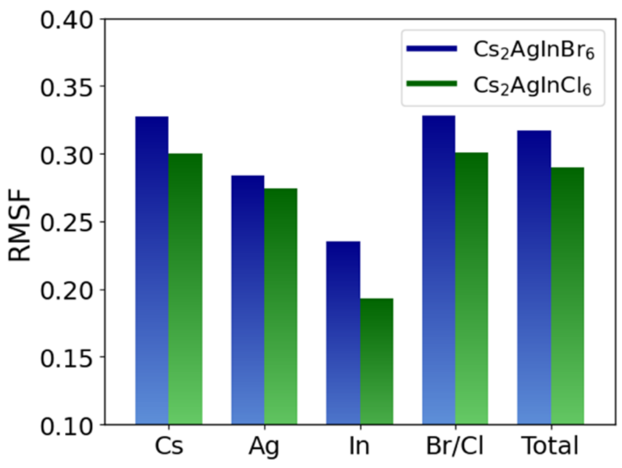
Non-Adiabatic Molecular Dynamics (NAMD)

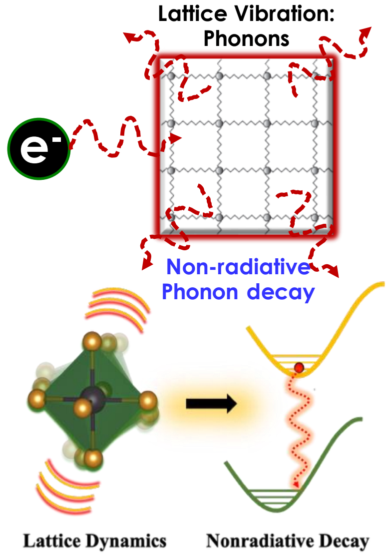
Charge carrier lifetime, Recombination rate, Excited state dynamics

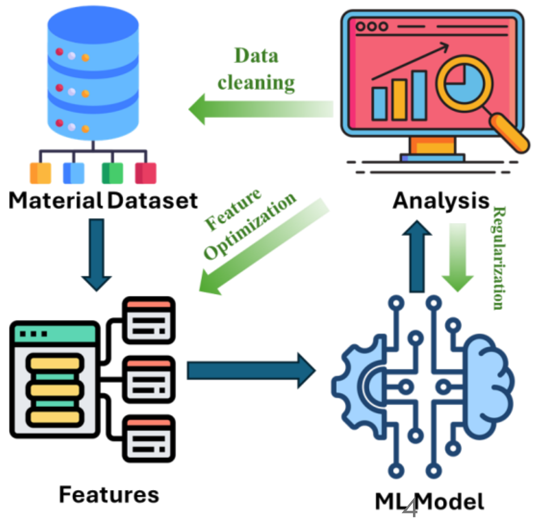
Machine Learning for materials

Supervised and Unsupervised Machine Learning









Ternary Selenides

1. Initial screening of Ternary selenides

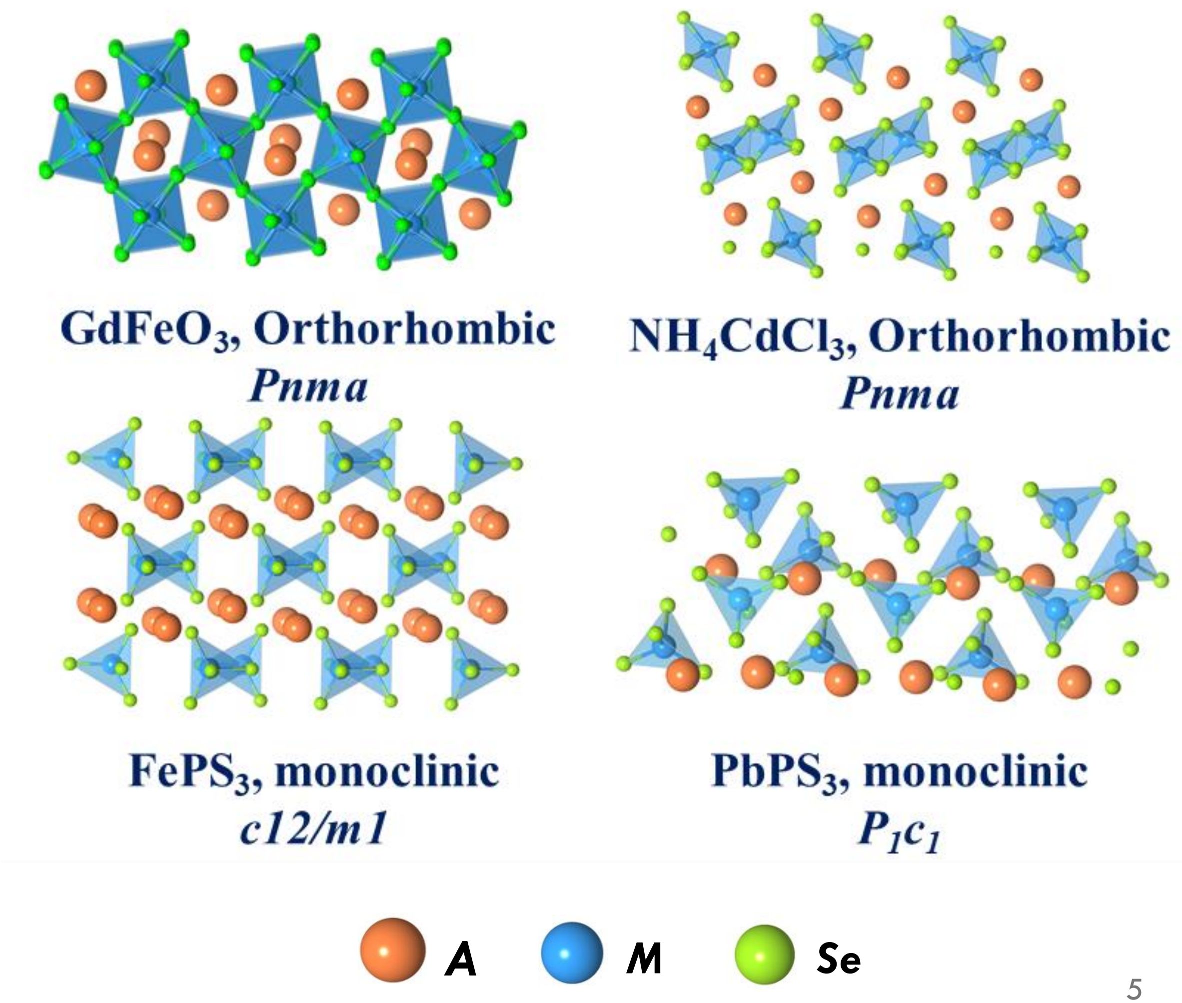
$AMSe_3$

54 × 53 = 2862 possible ternary selenides

Combinations for the Oxidation state of : 'A' and 'M'

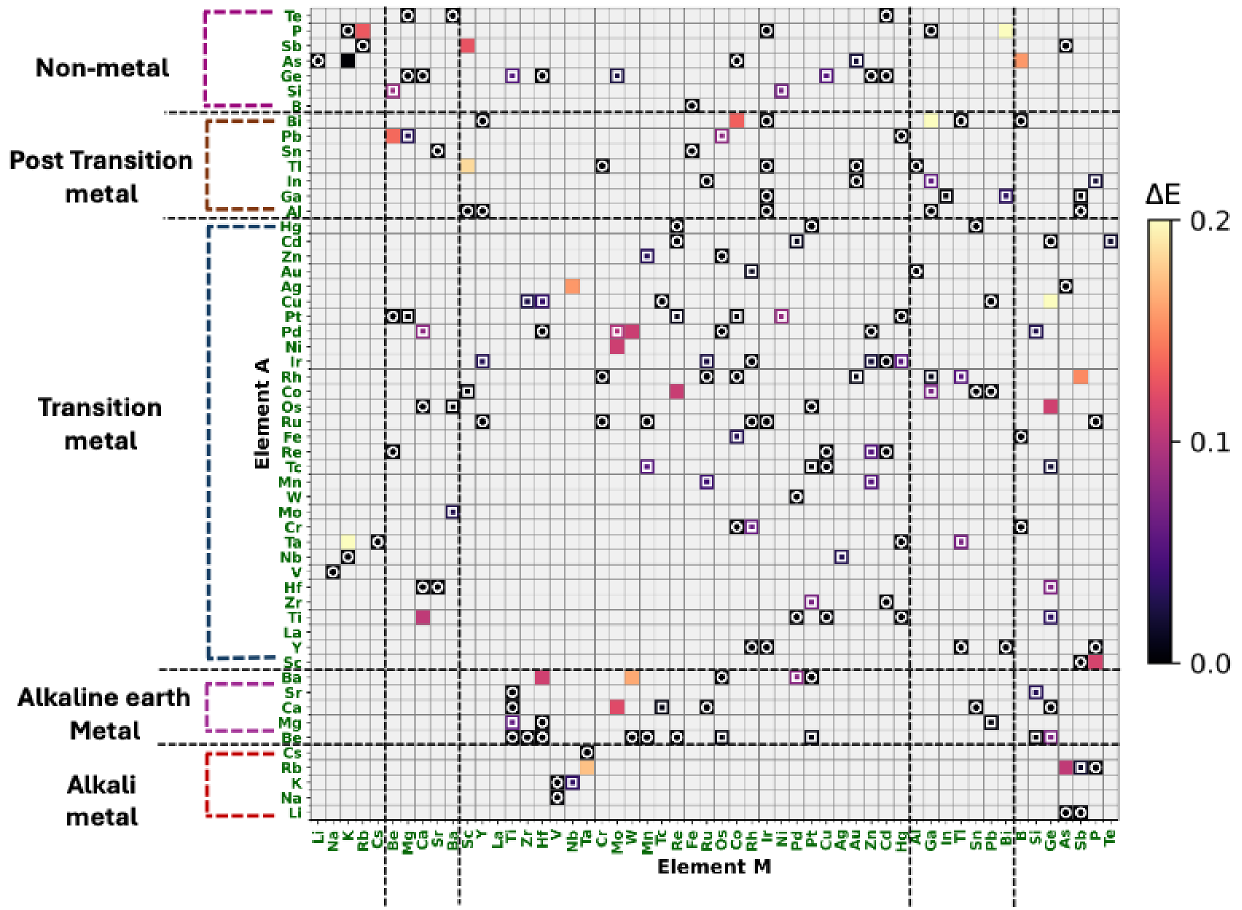
(+1, +5) (+2, +4) (+3, +3) (+4, +2) (+5, +1)

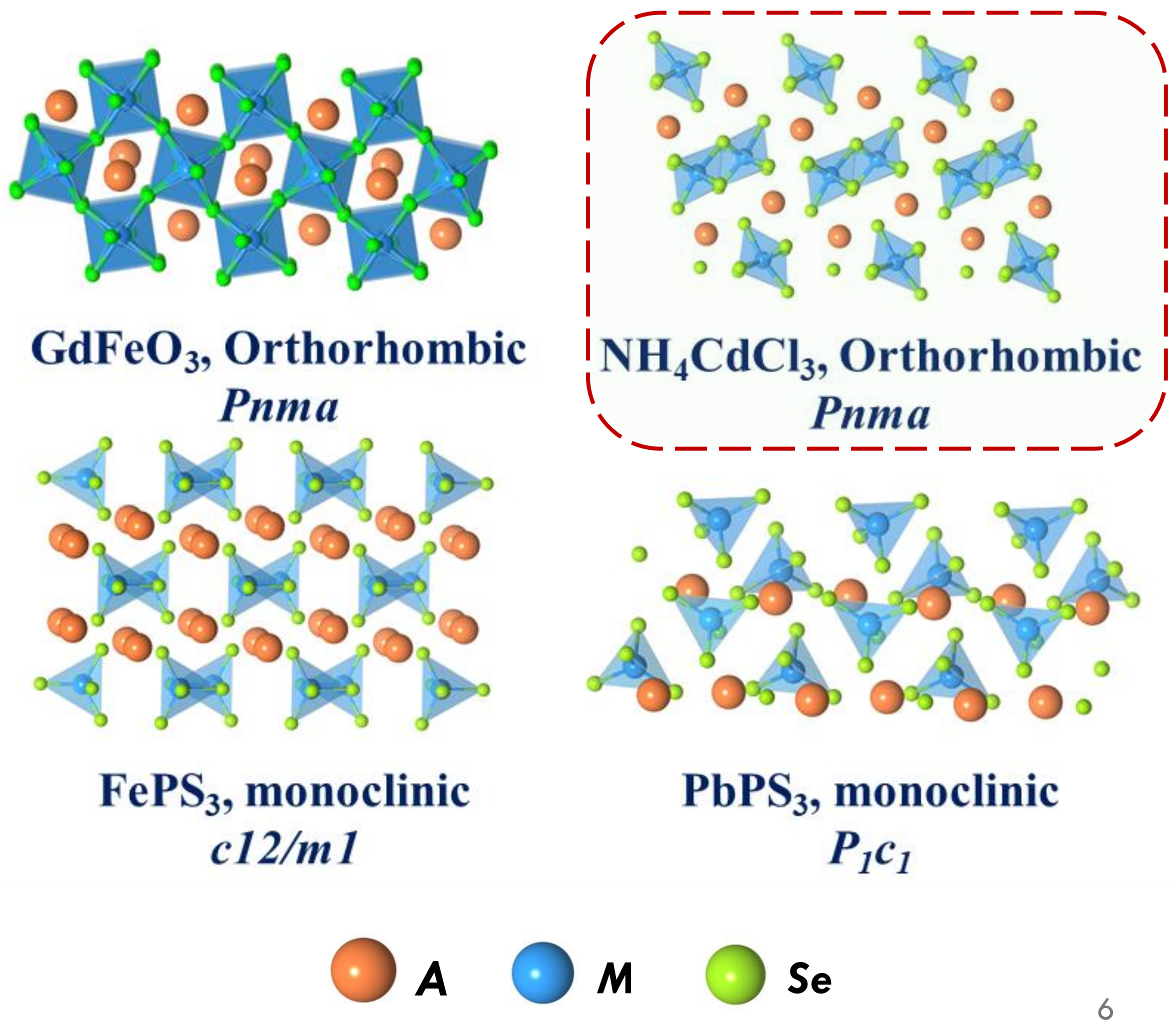
920 Final $AMSe_3$ candidates



Stability

2. Assessing Phase Stability





Stability

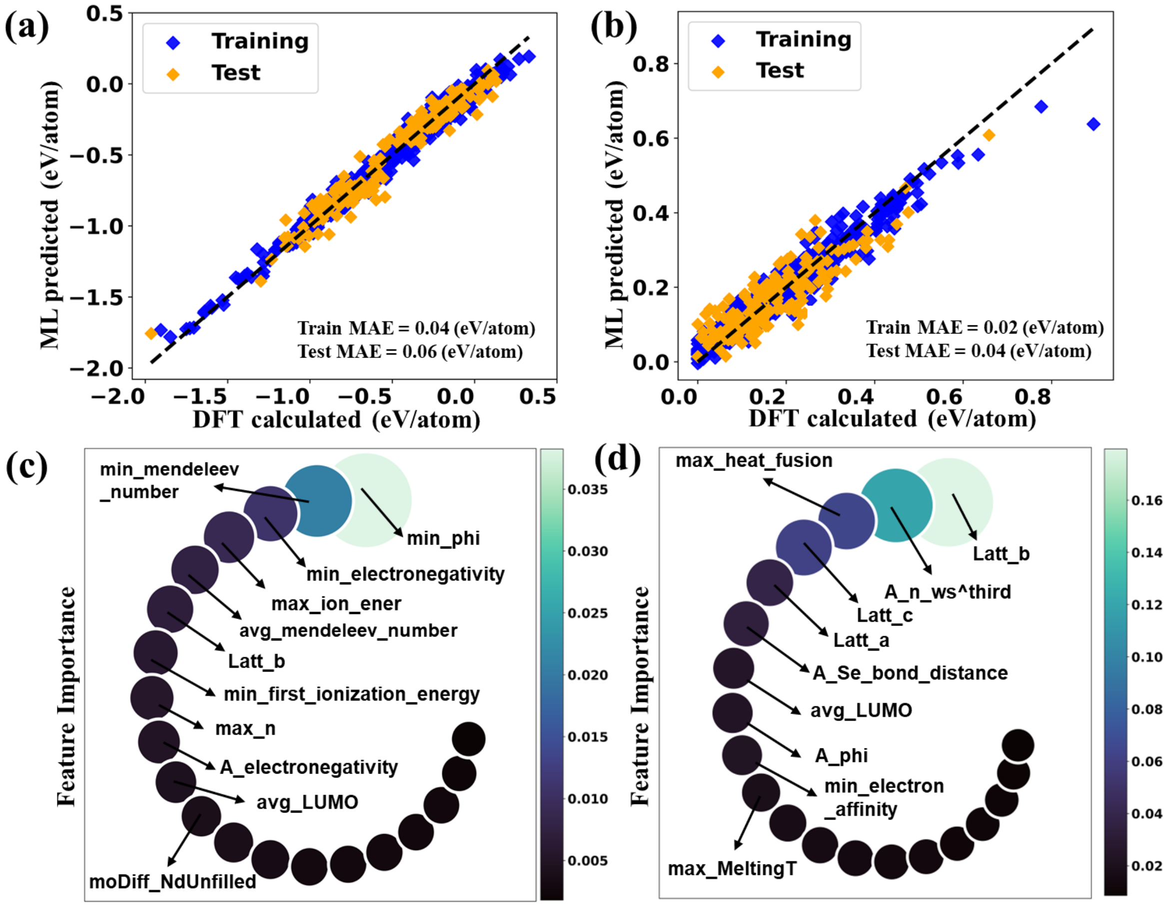
3. Assessing Thermodynamic stability

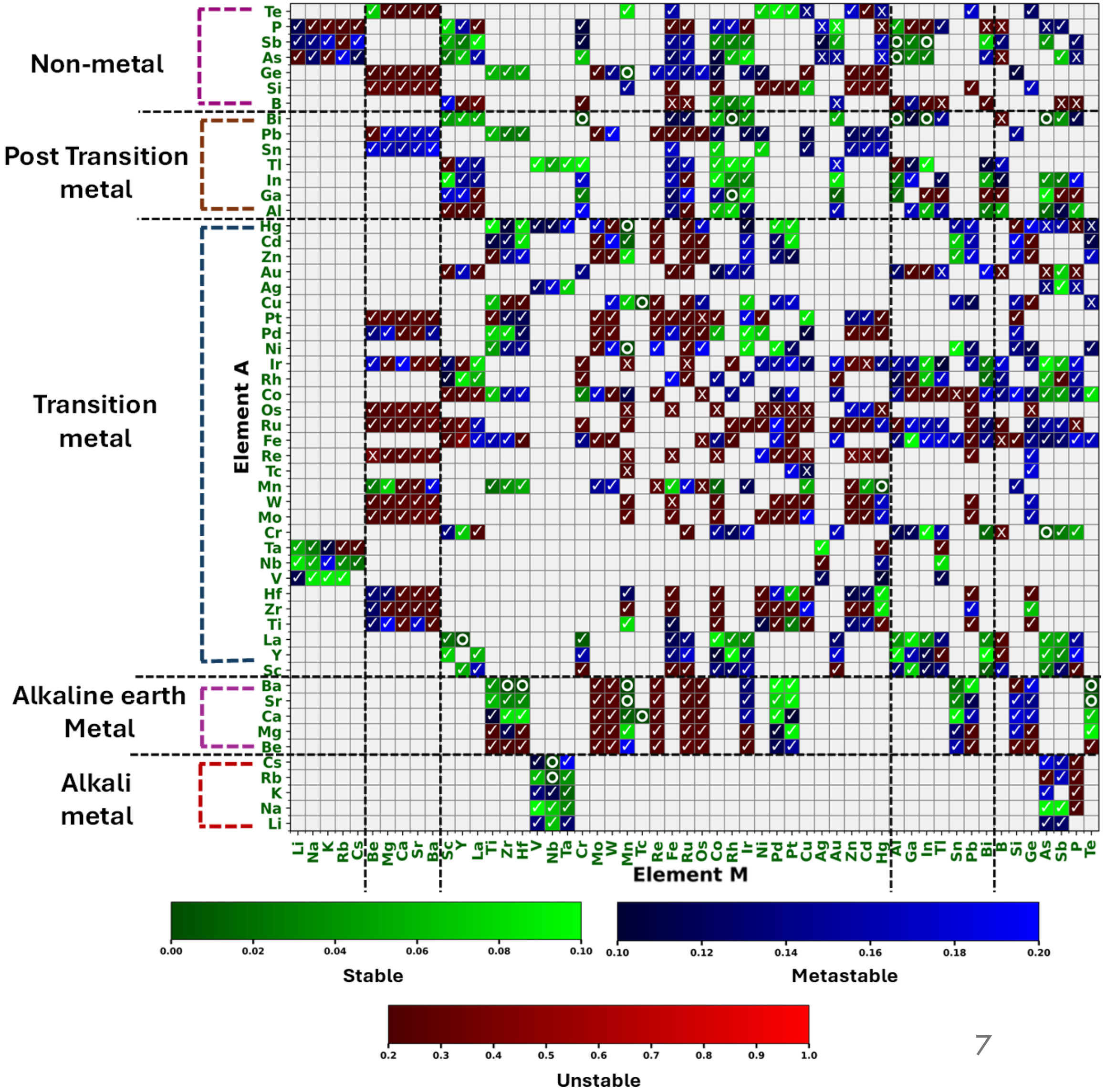
Screened candidates: 222

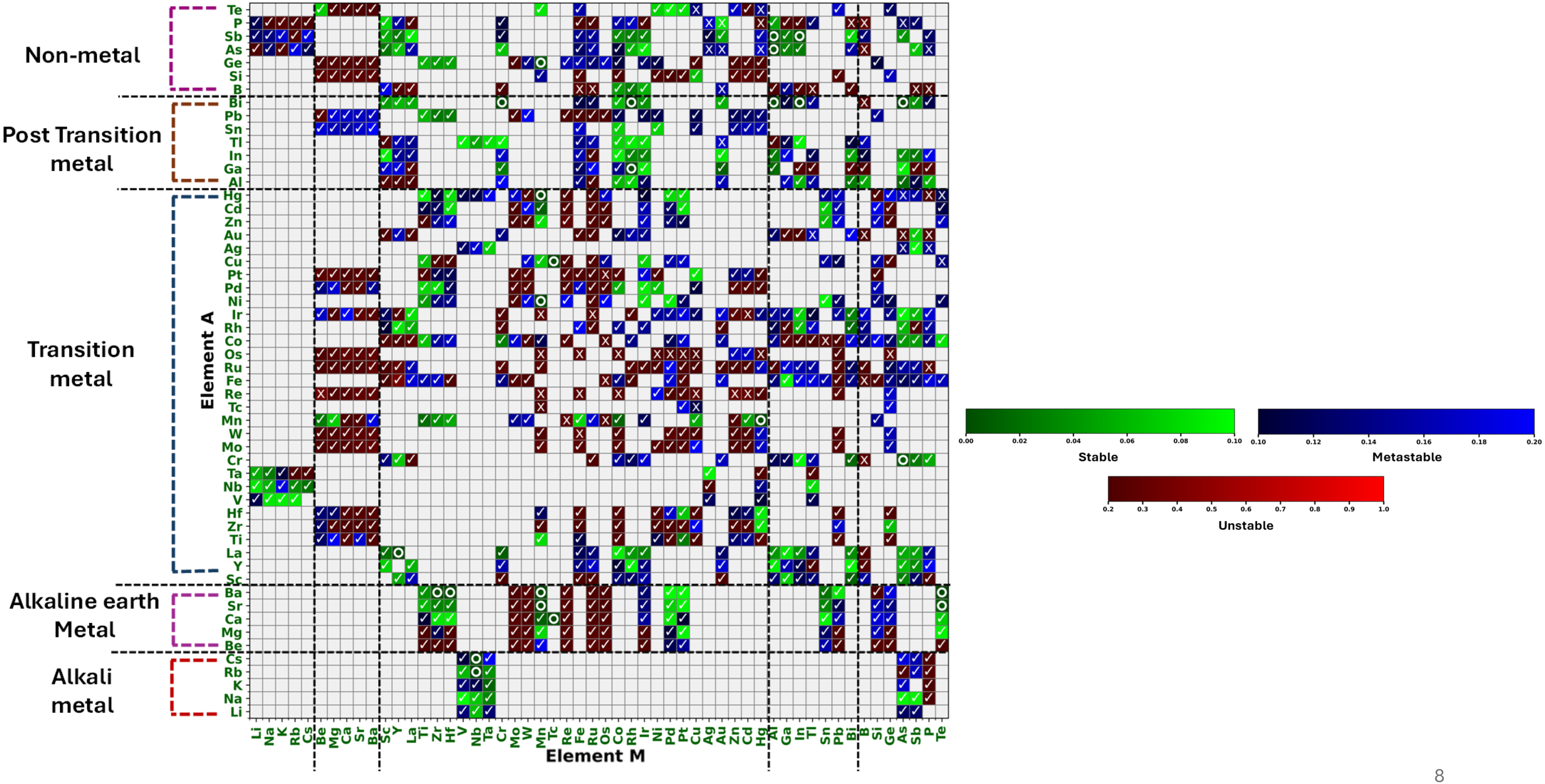
Criteria for Thermodynamic Stability

$E_{hull} < 0.1\ eV/atom$

$E_{form} \leq 0\ eV/atom$







Non-metal
Post Transition metal
Transition metal
Alkaline earth Metal
Alkali metal
Element A
Element M
Stable
Metastable
Unstable

Suitable Bandgap

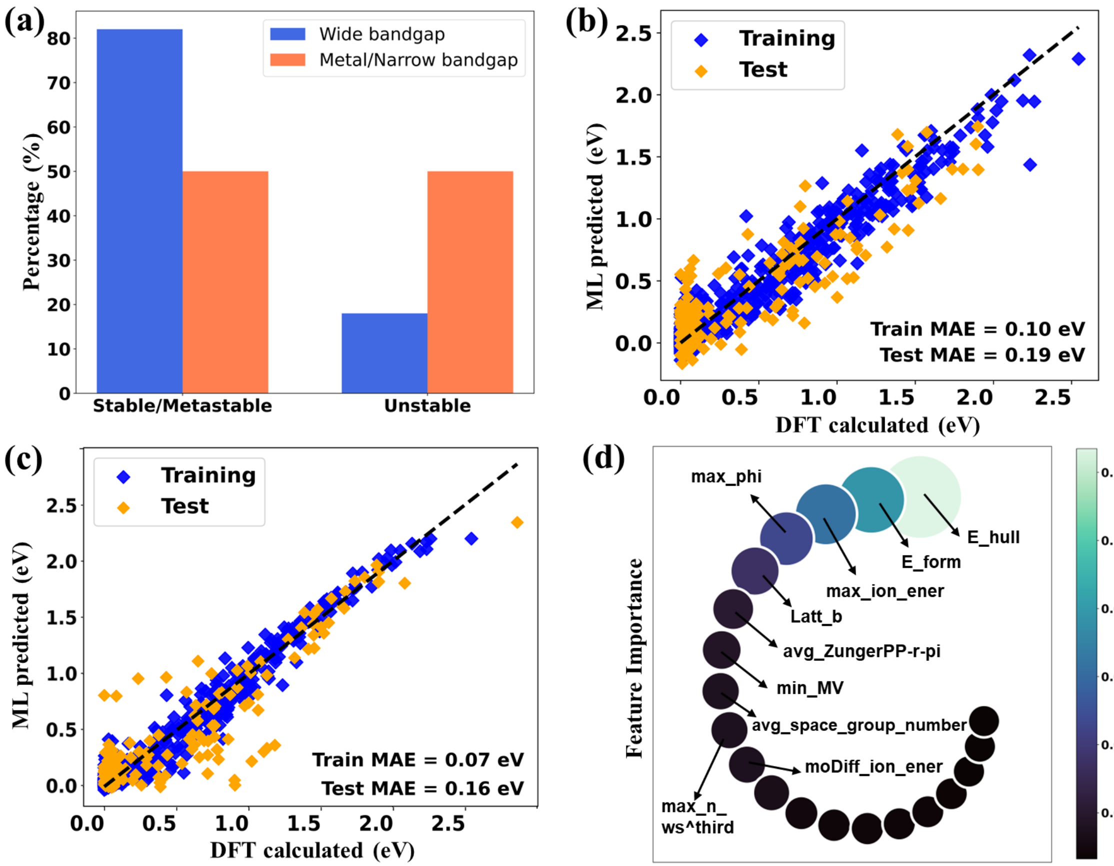
4. Screening based on Bandgap

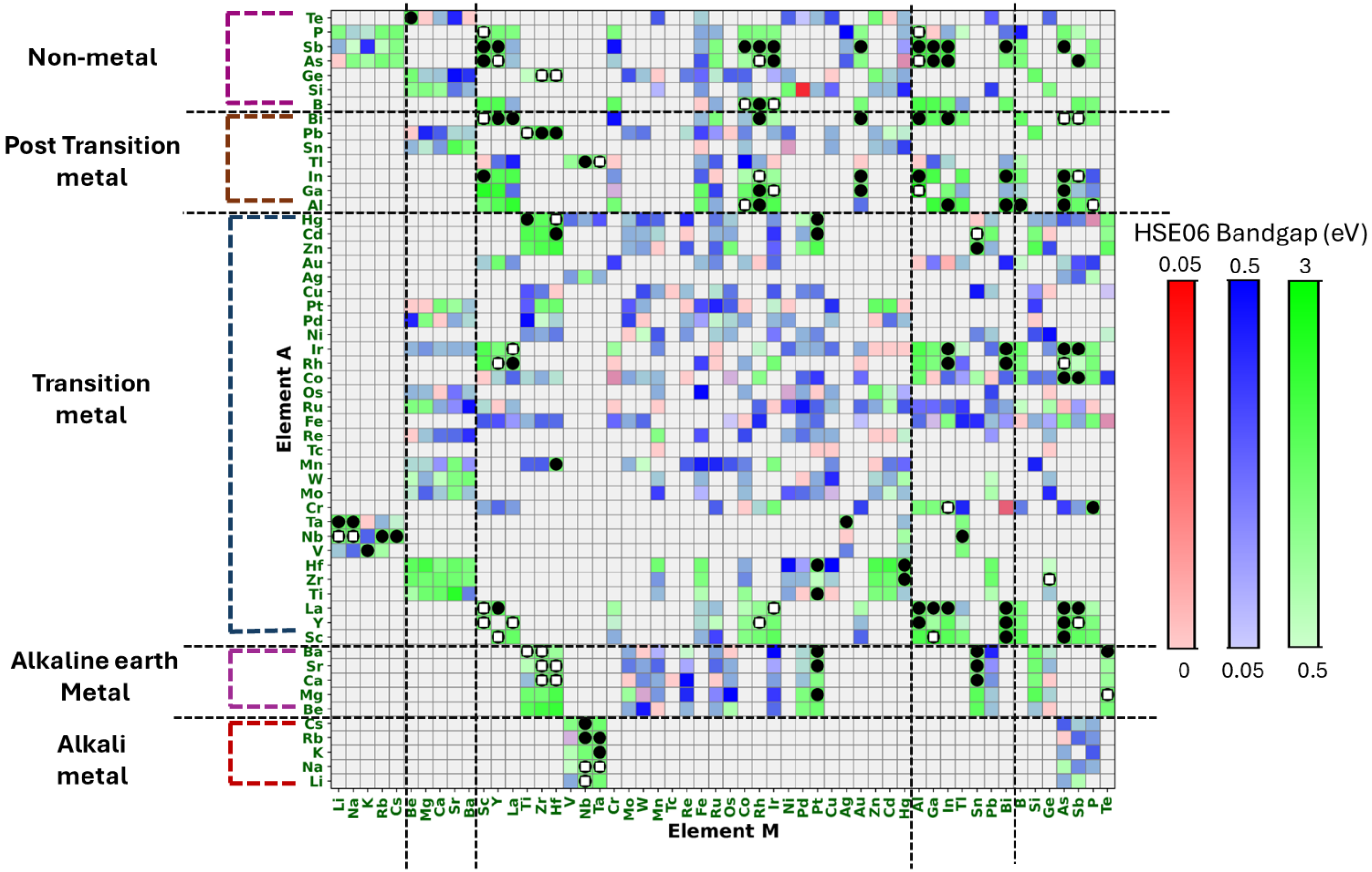
Screened candidates: 51

Criteria for Bandgap Screening

HSE06 Bandgap > 0.5 eV

(Direct Bandgap)

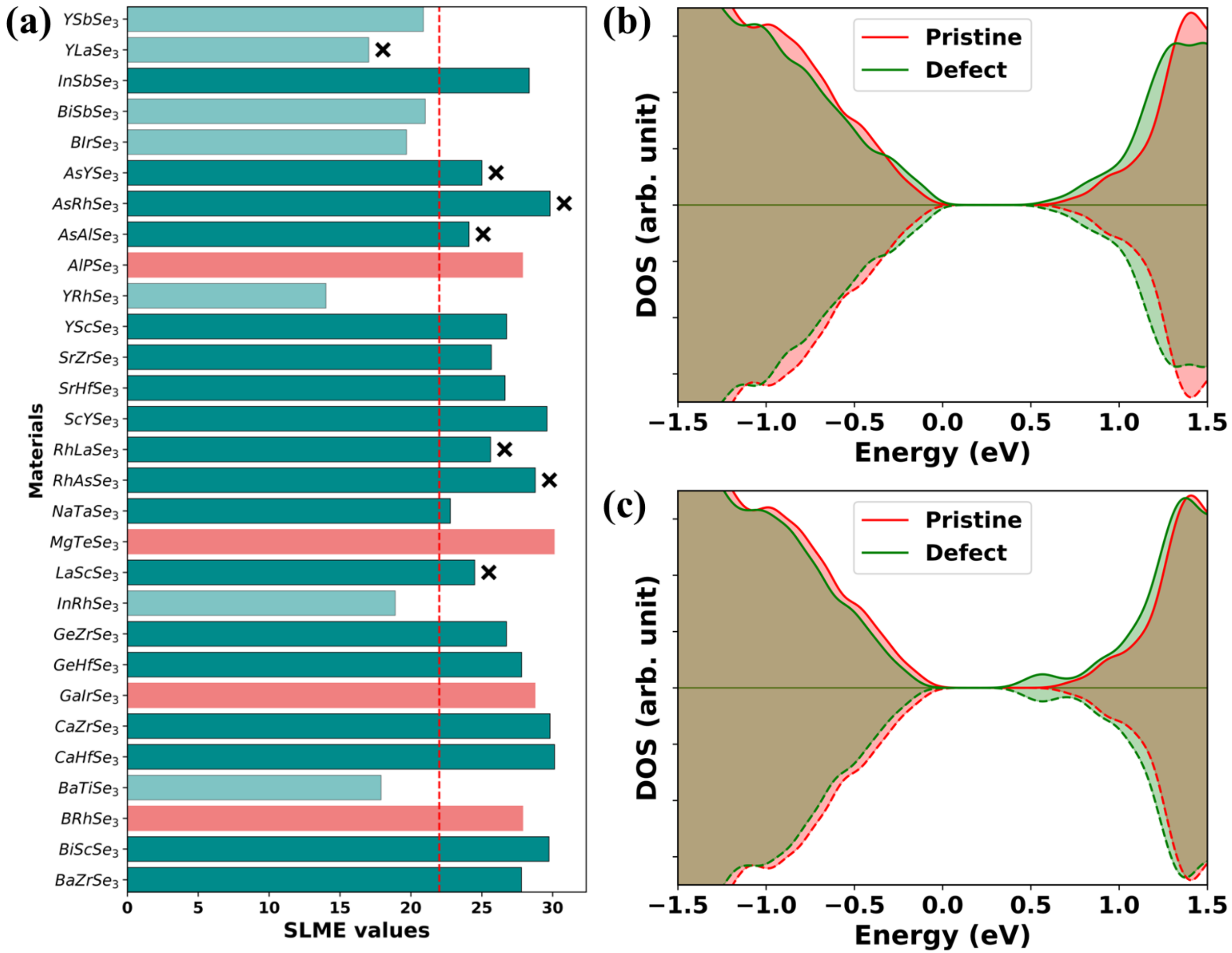




HT Screening

5. Screening based on Effective Masses → SLME + Phase stability → Toxicity → Defect Analysis

Screened candidates: 7



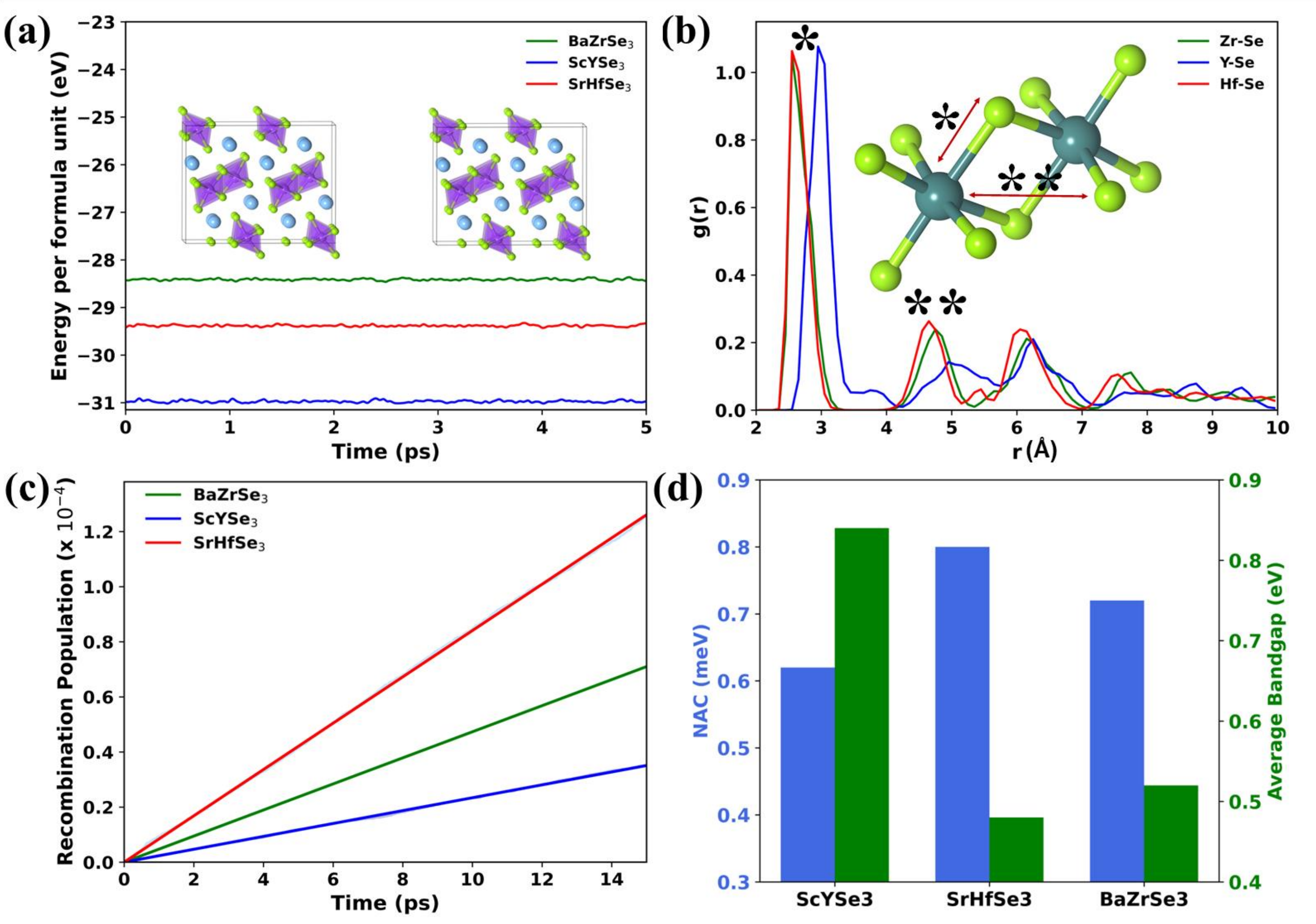
Criteria:

- ❑ Carrier Effective mass: $m_e < 0.1$ and $m_h < 0.1$
- ❑ SLME > 22%
- ❑ No Toxic Elements
- ❑ Defect Tolerance
- ❑ Phonon calculations

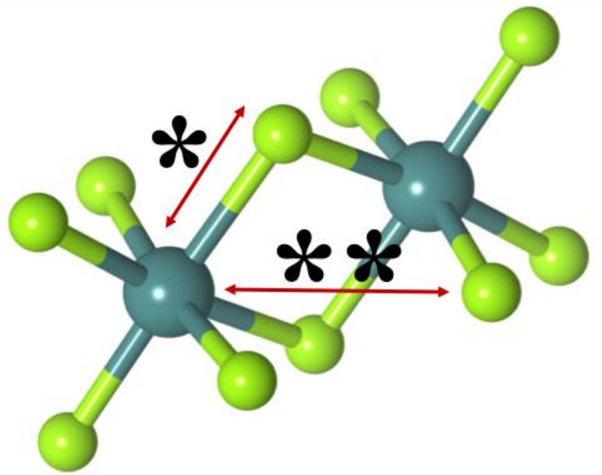
SLME (Spectroscopic Limited Maximum Efficiency)

The SLME is a theoretical photovoltaic energy conversion efficiency; it takes into account the effects of the material-dependent absorption coefficients from first-principles calculations and nonradiative recombination.

AIMD and NAMD

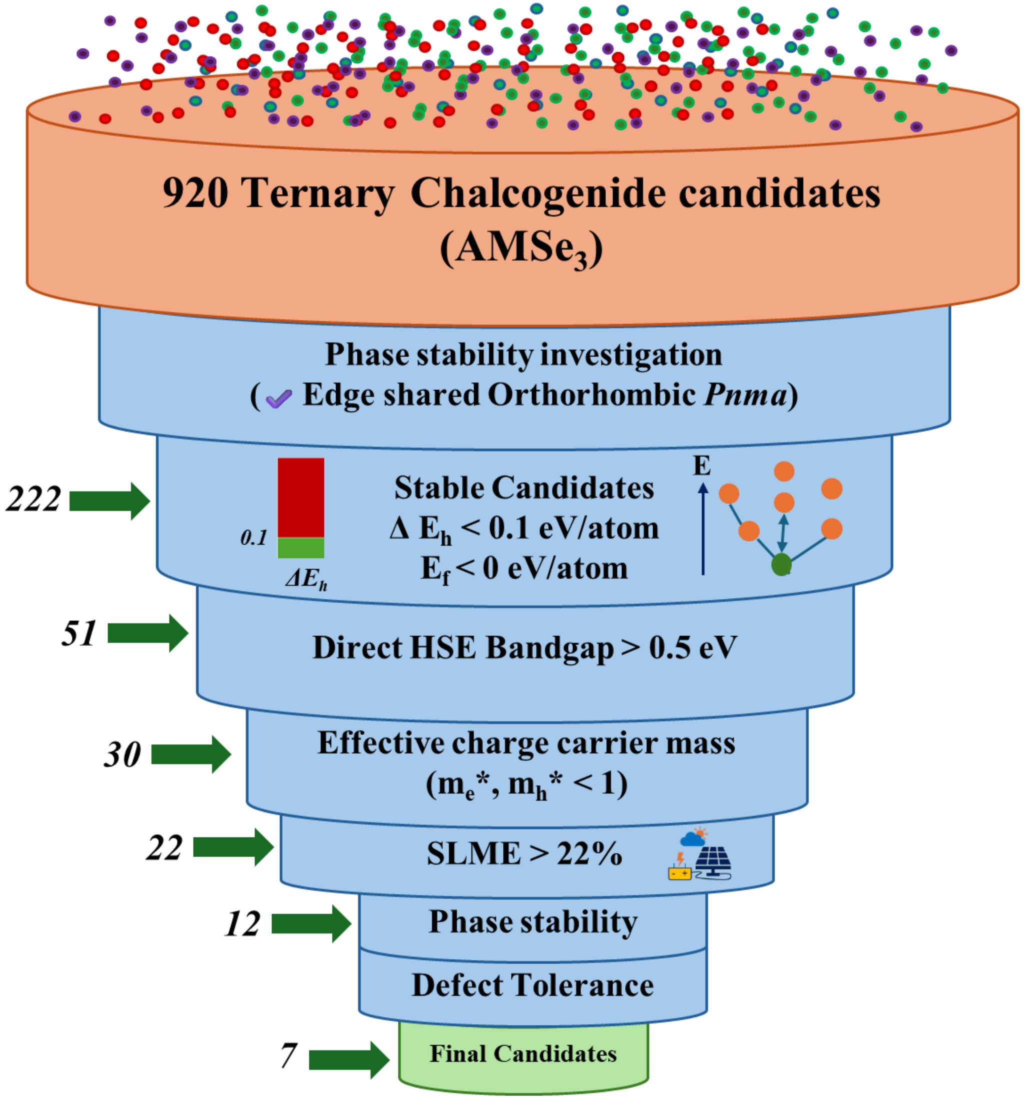


Material	Recombination Lifetime (ns)
$BaZrSe_3$	2.1
$ScYSe_3$	4.2
$SrHfSe_3$	1.18
$CsPbBr_3$[1]	1.45



[1]W. Li, A. S. Vasenko, J. Tang, O. V. Prezhdo, *The Journal of Physical Chemistry Letters* 2019, *10*, 6219.

Summary



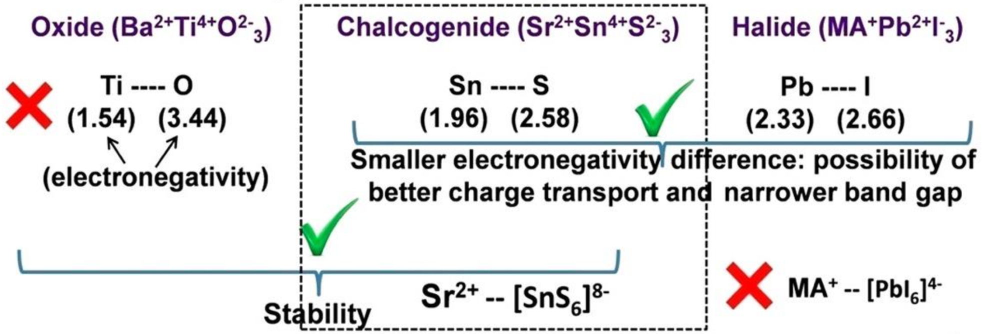
Seven Final $AMSe_3$ candidates

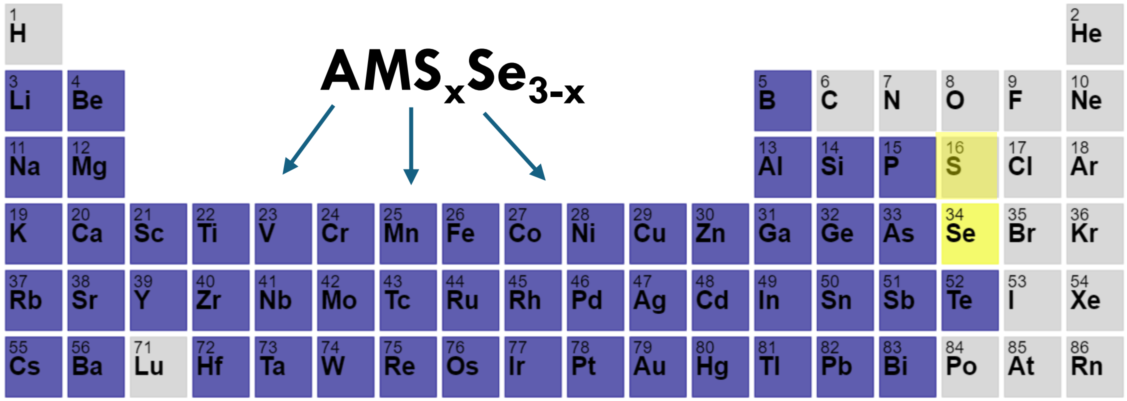
Compound	HSE06 Band gap (eV)	m_e^*	m_h^*	SLME (%) (1 μm)
$BaZrSe_3$	0.99	0.482	-0.587	27.80
$CaZrSe_3$	1.11	0.479	-0.306	29.81
$GeZrSe_3$	0.85	0.406	-0.525	26.74
$ScYSe_3$	1.43	0.569	-0.639	29.60
$SrHfSe_3$[1]	1.0	0.401	-0.536	26.64
$SrZrSe_3$[2]	0.84	0.968	-0.558	25.67
$YScSe_3$	0.96	0.679	-0.63	26.75

1. *Moroz et al.; Inorg. Chem.* 2018, 57, 12, 7402–7411
2. *Lee et al.; Solid State Sciences*, 2005, 7, 9, 1049-1054

Prospects

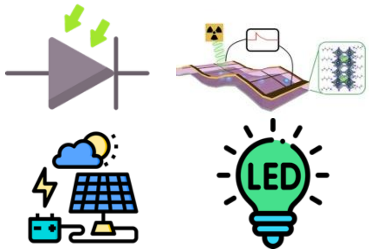
Scope of Chalcogenide Perovskite



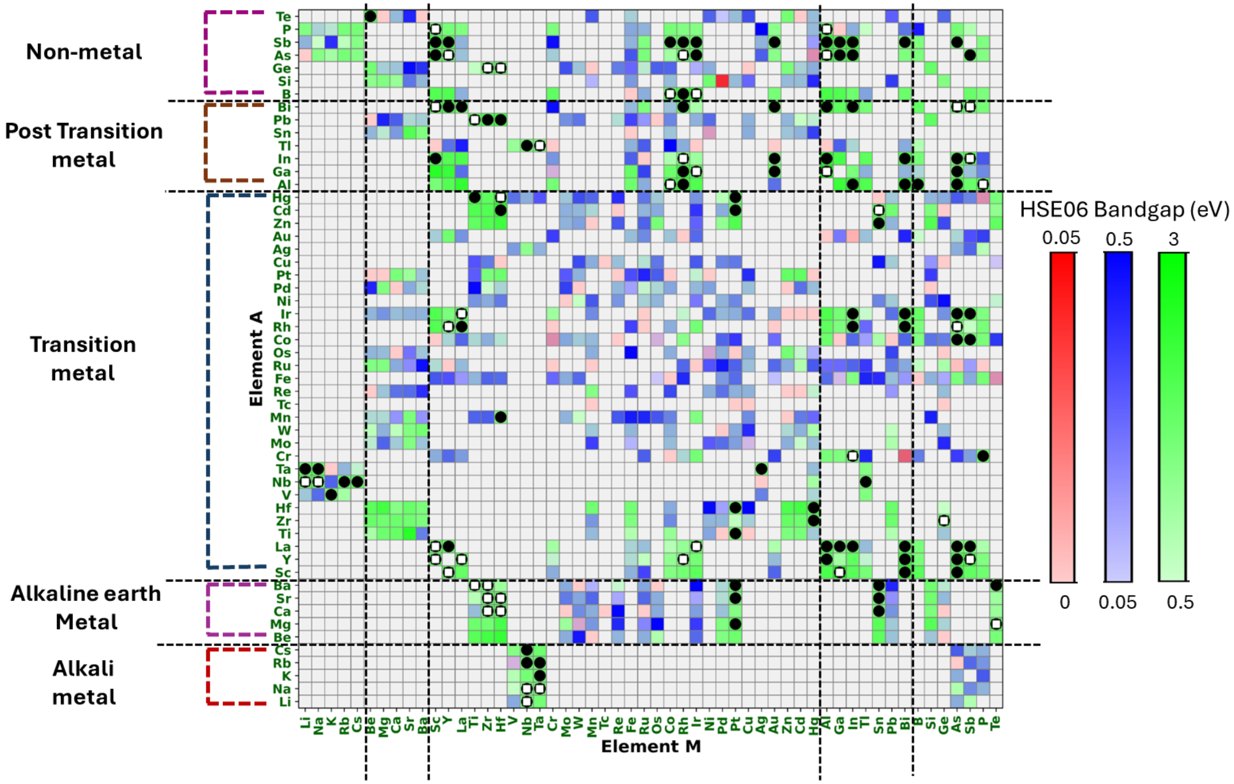


Research Gap

- Limited Exploration of Mixed-Anion Systems (S/Se)
- Defect study in Mixed-Anion Systems Remains Unmapped



Thermoelectrics?



What did we miss?

- Candidates with a Bandgap between 0.1 eV and 0.5 eV.
- We also ruled out all indirect bandgap candidates.

A Special Thanks

- I would like to acknowledge my PI, **Prof. Dibyajyoti Ghosh,** for his utmost support and guidance.
- My sincere gratitude towards the CDFM lab members.
- I would like to acknowledge IIT Delhi for HPC resources
- I thank my friends and family.

Want to read?

Issue 13, 2025

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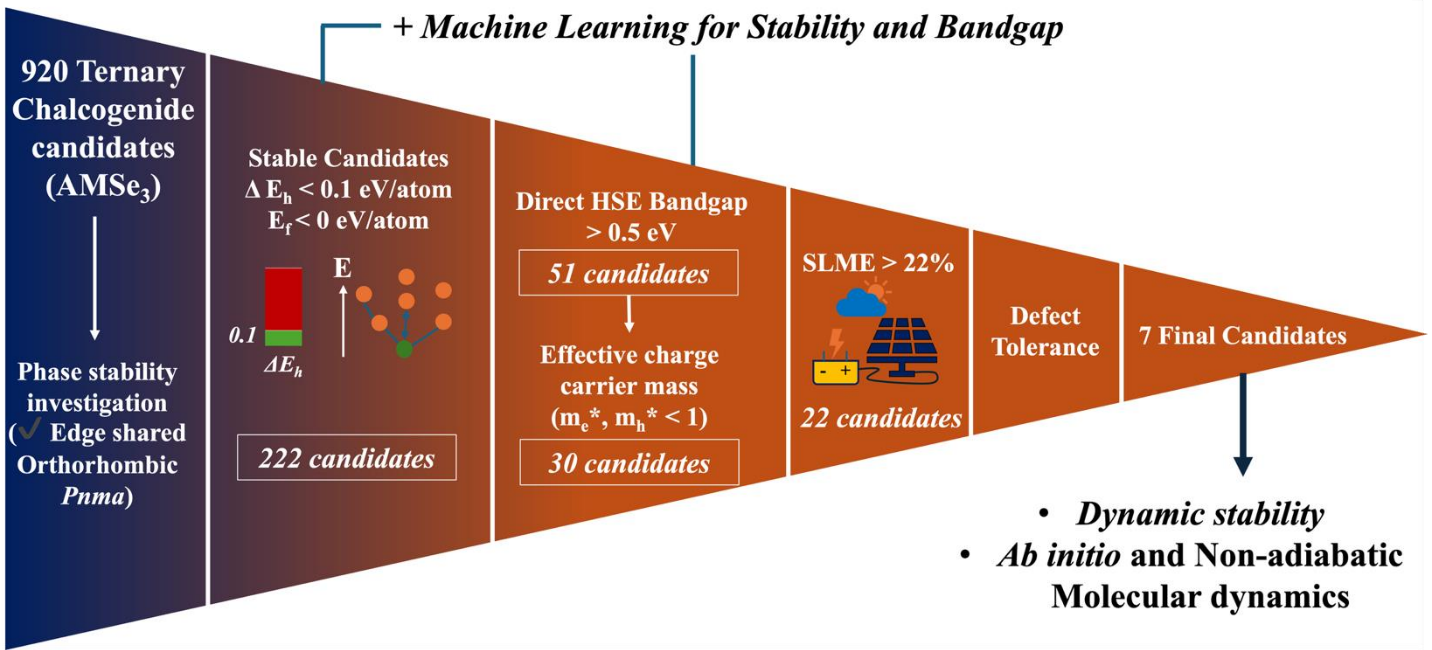
From the journal:
Journal of Materials Chemistry A

High-throughput and data-driven search for stable optoelectronic $AMSe_3$ materials†

Check for updates

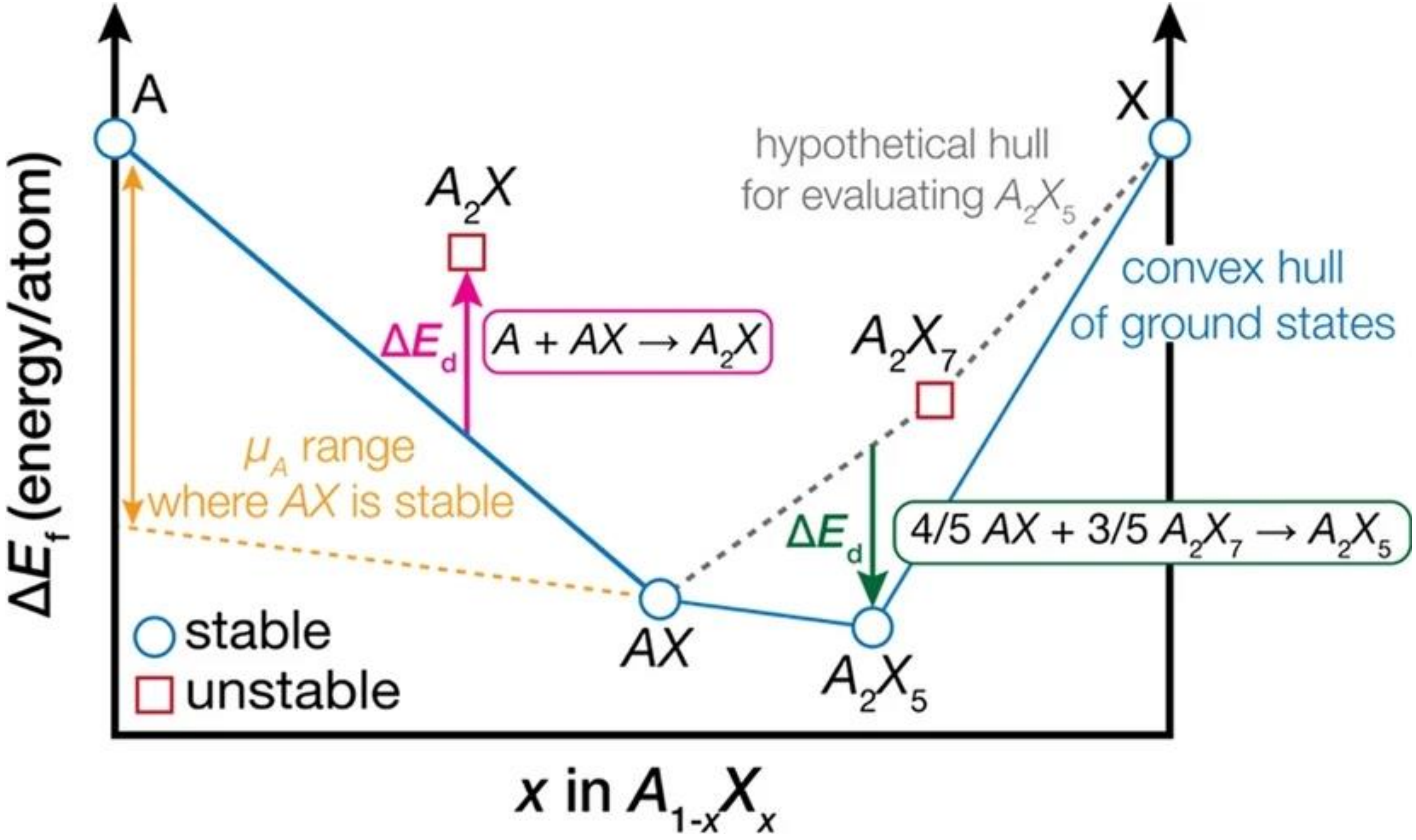
Nikhil Singh, ‡[a] Kushal Samanta, ‡[b] Suneet K. Maharana, [c] Koushik Pal, [d] Sergei Tretiak, [e] Anjana Talapatra [f] and Dibyajyoti Ghosh *[ab]



Thank

You

E_{hull}


A
X
hypothetical hull
for evaluating A_2X_5
A_2X
convex hull
of ground states
ΔE_d
$A + AX \rightarrow A_2X$
A_2X_7
μ_A range
where AX is stable
ΔE_d
$4/5\ AX + 3/5\ A_2X_7 \rightarrow A_2X_5$
ΔE_f (energy/atom)
stable
unstable
AX
A_2X_5
x in $A_{1-x}X_x$