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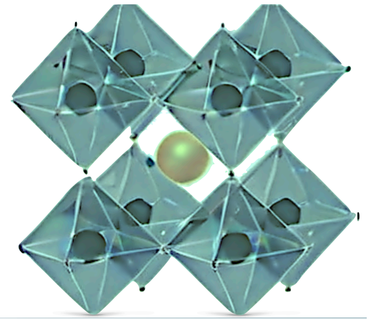

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FUNCTIONAL MATERIALS GROUP

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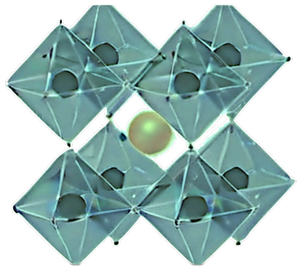

DEVELOPMENT OF ARTIFICIAL INTELLIGENCE - BASED MODEL FOR SIMULATION, SYNTHESIS AND STABILIZATION OF THE NEXT GENERATION SOLAR CELL AND DISPLAY MATERIALS: THE PEROVSKITES

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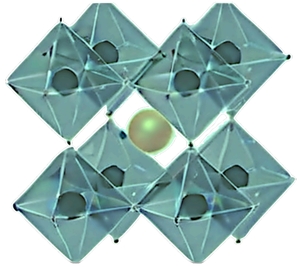
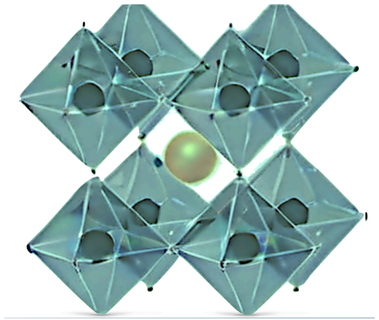
Institute of Chemical Physics



ԱՐՀԵՍՏԱԿԱՆ ԲԱՆԱԿԱՆՈՒԹՅԱՆ ՎՐԱ ՀԻՄՆՎԱԾ ՄՈԴԵԼԻ ՄՇԱԿՈՒՄ ՀԱՋՈՐԴ ՍԵՐՆԴԻ ԱՐԵՎԱՅԻՆ ԲՋԻՋՆԵՐԻ և ԴԻՍՓԼԵՅՆԵՐԻ ՆՅՈՒԹԵՐԻ ՄՈԴԵԼԱՎՈՐՄԱՆ, ՍԻՆԹԵԶՆԵՐԻ և ԿԱՅՈՒՆԱՑՄԱՆ ՀԱՄԱՐ. ՊԵՐՈՎՍԿԻՏՆԵՐ



FUNCTIONAL MATERIALS GROUP'S ACHIEVEMENTS IN 2025

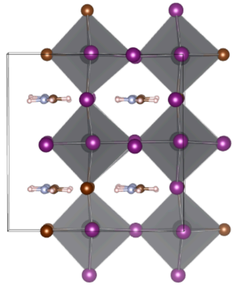
Team

1. Hayk Khachatryan
2. Arevik Asatryan
3. Sadegh Kaviani
4. Sona Grigoryan
5. Nane Petrosyan
6. Gurgen Kolotyan
7. Vahe Hovhannisyan
8. Alik Madoyan
9. Susanna Atoyan

Objectives

1. Find new perovskite materials through combined ML, DFT, MD and experimental methods.

ABX_3



A. For solar cell applications.
B. For display applications.

2. Improve ML methodology continuously.

3. Based on the gained experience expand the study towards other functional materials

Simple dataset - simple algorithms

1. 110 unique data
2. Limited elements - up to 7
3. Source data contained 5 columns (3 calculated ionic radii for A, B, X sites, T_f, E_g)
4. Simple ML algorithms - train, validate, test, evaluation
5. Generation of the new data of 44000
6. Prediction of Eg
7. DFT
8. Experiments
9. Validation

Filtered 9, DFT validated 9, experimentally validated 1

$$FAPb(Br_{0.375}I_{0.625})_3$$

ELSEVIER

Materials & Design

Volume 260, December 2025, 114902

Accelerated composition optimization of hybrid perovskites via data-driven materials design, DFT calculations and synthesis

Sona Grigoryan [a], Nane Petrosyan [a b], Gurgen Kolotyan [a], Arpine Kozmanyan [a], Varazdat Avetisyan [a], Hayk Zakaryan [b], Michael J. Schöning [c], Arevik Asatryan [a] ✉, Hayk Khachatryan [a]

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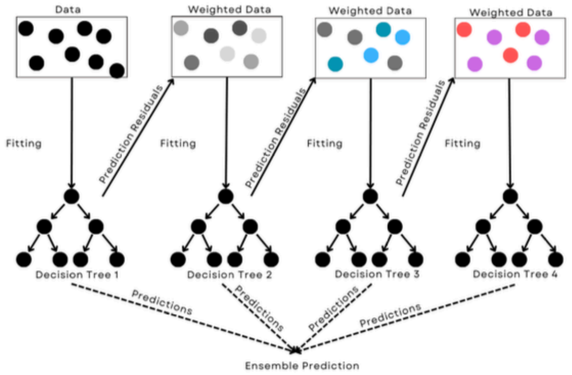
Validation of 3 parameters: Crystal structure, Band gap energy, stability

Data collection

x A	yA	zA	rA	rB	xC	yC	zC	rC	TF	Eg
0	1	0	2.16	1.19	1	0	0	1.81	0.94	3.07
0	1	0	2.16	1.19	0.67	0.33	0	1.86	0.92	2.85
0	1	0	2.16	1.19	0.05	0.95	0	1.95	0.93	2.33
1	0	0	1.67	1.19	0	0.6	0.4	2.06	0.81	1.77
0.1	0.15	1.75	2.39	1.19	0	0.17	0.83	2.16	0.96	1.62
...	...									

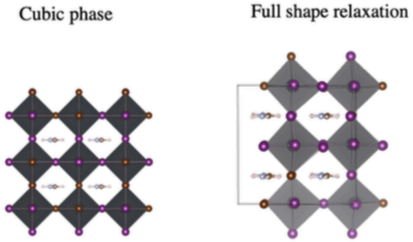
ML algorithms



Data Filtration to Data Generation

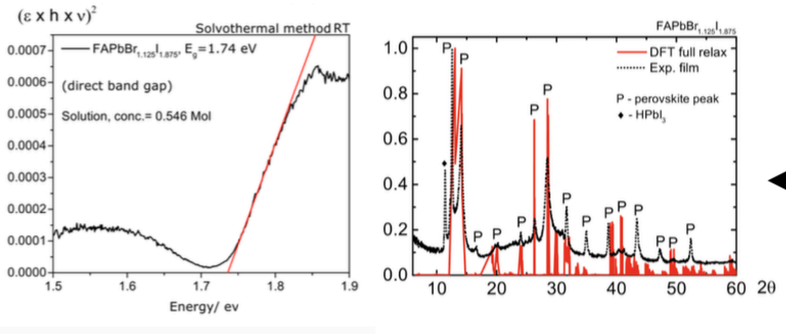
Composite	Ionic radius of A cation/Å	Ionic radius of B metal/Å	Ionic radius of C halide/Å	Calculated tolerance factor	predicted by Gradient Boosting / ev	predicted by Random Forest / ev	predicted by Linear Regression / ev	calculated by DFT (GGA)/ ev	calculated by DFT+U/ ev
$FAPb(Cl_{0.25}Br_{0.375}I_{0.375})_3$	2.53	1.19	2.12	0.9933	1.61	1.61	1.74	1.74	
$FAPb(Cl_{0.25}Br_{0.25}I_{0.50})_3$	2.53	1.19	2.09	0.9959	1.69	1.69	1.83	1.67	
$FAPb(Cl_{0.25}Br_{0.125}I_{0.625})_3$	2.53	1.19	2.07	0.9975	1.68	1.68	1.96	1.79	
$FAPb(Cl_{0.25}Br_{0.25}I_{0.5})_3$	2.53	1.19	2.04	1.0002	1.82	1.76	2.05	1.82	
$FAPb(Cl_{0.25}Br_{0.125}I_{0.625})_3$	2.53	1.19	2.02	1.0019	2.04	1.91	2.18	1.93	
$FAPb(Cl_{0.25}Br_{0.25}I_{0.5})_3$	2.53	1.19	2.06	0.9985	1.81	1.79	1.92	1.75	
$FAPb(Cl_{0.5}I_{0.5})_3$	2.53	1.19	2.10	0.9949	1.57	1.64	1.87	1.71	
$FAPb(Cl_{0.5}I_{0.5})_3$	2.53	1.19	2.05	0.9992	1.64	1.70	2.09	1.89	

DFT calculations/ verification



Synthesis

Identification, characterization



Nanyang Technological University (NTU) showed $Cs_{0.15}FA_{0.85}PbI_{2.8}Cl_{0.2}$ reached 25.1% efficiency and retained over 93% after 1,000 h, and 98% after 1,100 h at 85 °C.

$FAPb(Br_{0.375}I_{0.625})_3$ by FMG has cubic crystal ($T_f = 0.99$), promising high efficiency (due to $E_g = 1.74\ eV$) and is **stable for more than a year in ambient conditions**, and it resists wide temperatures range 10-150 ºC, high humidity: 54% → material stability due to crystal stability.

Directions

1. Improvement and deepening of ML methods, applications.

   A. Material science → new perovskites
   B. Film optimization and other…

2. MD simulations for stability evaluation, interactions, etc.

   Searching for lead free perovskites utilizing DFT calculations.

3. Optimization of synthesis, preparation, stabilization and maintenance of precursors, perovskites, films

- Lead free perovskite solar cell

- Lead free perovskite for application in display materials

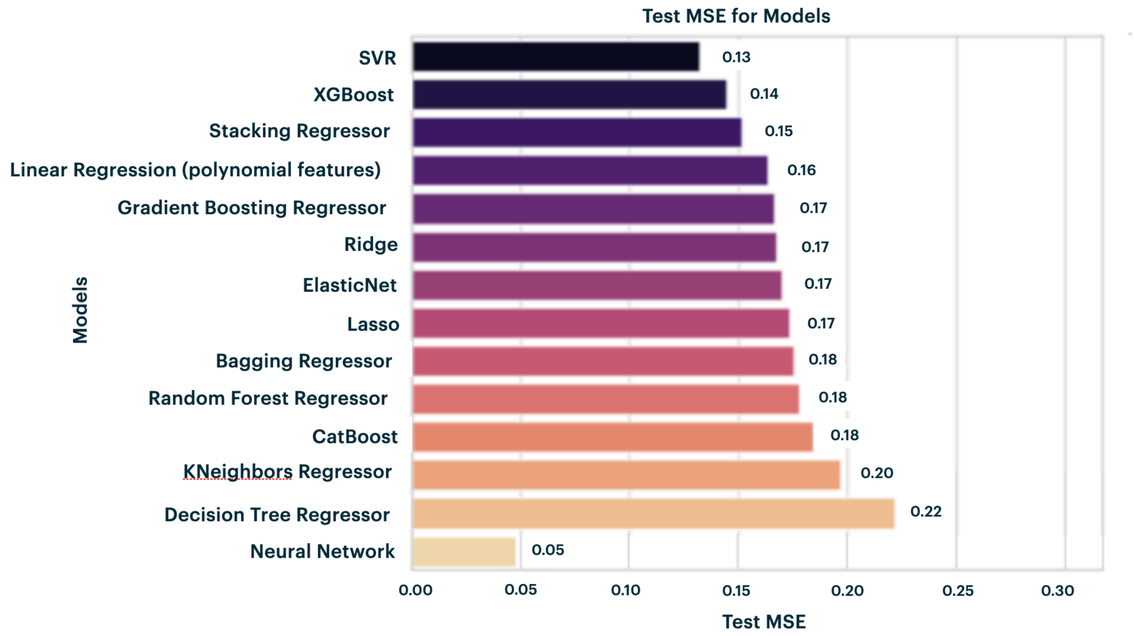
Complicated problems - deep learning: **Lead free perovskites**

1. **320 unique data (**1500**)**, ≈**600** after 1% Gaussian noise was added
2. Number of elements - up to 35
3. Source data contained 5 columns (3 calculated ionic radii for A, B, X sites, T_f, E_g)
4. NN and Simple ML algorithms- train, validate, test, evaluation
5. Generation of the new data - 3 mln.
6. Prediction of E_g
7. DFT
8. Experiments
9. Validation

Data collection/ organization with multicomponent perovskites	ML application on the data for E_g prediction, model selection	Data generation, T_f calculation, E_g prediction	Filtration based on crystal structure (T_f), and E_g	DFT stability calculation, further filtration	Synthesis, characterization, experimental validation	Film preparation optimization	Lead free stable, efficient perovskite for solar cells

Comparison of the models, NN predicted and filtered data

Performance difference between N and simple algorithms



Perovskite	Tolerance factor	Predicted E_g
$MA_{0.750}FA_{0.250}Bi_{0.875}Sb_{0.125}(I_{0.625}Se_{0.375})_3$	0.91	2.55
$MA_{0.750}FA_{0.250}Bi_{0.750}Sb_{0.250}(I_{0.625}Se_{0.375})_3$	0.90	2.50
$MA_{0.625}FA_{0.375}Bi_{0.875}Sb_{0.125}(I_{0.625}Se_{0.375})_3$	0.92	2.57
$MA_{0.625}FA_{0.375}Bi_{0.750}Sb_{0.250}I_{0.625}Se_{0.375})_3$	0.91	2.52
$MA_{0.625}FA_{0.375}Bi_{0.625}Sb_{0.375}I_{0.625}Se_{0.375})_3$	0.91	2.45
$MA_{0.500}FA_{0.500}Bi_{0.875}Sb_{0.125}(I_{0.625}Se_{0.375})_3$	0.94	2.57
$MA_{0.500}FA_{0.500}Bi_{0.750}Sb_{0.250}I_{0.625}Se_{0.375})_3$	0.93	2.52
$MA_{0.500}FA_{0.500}Bi_{0.625}Sb_{0.375}I_{0.625}Se_{0.375})_3$	0.92	2.46
$MA_{0.500}FA_{0.500}Bi_{0.500}Sb_{0.500}I_{0.625}Se_{0.375})_3$	0.91	2.39
$MA_{0.500}FA_{0.500}Bi_{0.375}Sb_{0.625}I_{0.625}Se_{0.375})_3$	0.90	2.31
$MA_{0.375}FA_{0.625}Bi_{0.875}Sb_{0.125}(I_{0.625}Se_{0.375})_3$	0.95	2.57
$MA_{0.375}FA_{0.625}Bi_{0.750}Sb_{0.250}(I_{0.625}Se_{0.375})_3$	0.94	2.52
$MA_{0.375}FA_{0.625}Bi_{0.625}Sb_{0.375}(I_{0.625}Se_{0.375})_3$	0.93	2.46
$MA_{0.375}FA_{0.625}Bi_{0.500}Sb_{0.500}(I_{0.625}Se_{0.375})_3$	0.92	2.40
$MA_{0.375}FA_{0.625}Bi_{0.375}Sb_{0.625}(I_{0.625}Se_{0.375})_3$	0.91	2.32
$MA_{0.375}FA_{0.625}Bi_{0.250}Sb_{0.750}(I_{0.625}Se_{0.375})_3$	0.91	2.18
$MA_{0.250}FA_{0.750}Bi_{0.875}Sb_{0.125}(I_{0.625}Se_{0.375})_3$	0.96	2.57
$MA_{0.250}FA_{0.750}Bi_{0.750}Sb_{0.250}(I_{0.625}Se_{0.375})_3$	0.95	2.52
$MA_{0.250}FA_{0.750}Bi_{0.625}Sb_{0.375}(I_{0.625}Se_{0.375})_3$	0.94	2.46
$MA_{0.250}FA_{0.750}Bi_{0.500}Sb_{0.500}(I_{0.625}Se_{0.375})_3$	0.93	2.40
$MA_{0.250}FA_{0.750}Bi_{0.375}Sb_{0.625}(I_{0.625}Se_{0.375})_3$	0.93	2.33
$MA_{0.250}FA_{0.750}Bi_{0.250}Sb_{0.750}(I_{0.625}Se_{0.375})_3$	0.92	2.18
$MA_{0.250}FA_{0.750}Bi_{0.125}Sb_{0.875}(I_{0.625}Se_{0.375})_3$	0.91	2.06
$MA_{0.125}FA_{0.875}Bi_{0.875}Ag_{0.125}(I_{0.750}Se_{0.250})_3$	**0.90**	**2.42**
$MA_{0.125}FA_{0.875}Bi_{0.875}Sb_{0.125}(I_{0.625}Se_{0.375})_3$	0.98	2.58
$MA_{0.125}FA_{0.875}Bi_{0.750}Sb_{0.250}(I_{0.625}Se_{0.375})_3$	0.97	2.52
$MA_{0.125}FA_{0.875}Bi_{0.625}Sb_{0.375}(I_{0.625}Se_{0.375})_3$	0.96	2.47
$MA_{0.125}FA_{0.875}Bi_{0.500}Sb_{0.500}(I_{0.625}Se_{0.375})_3$	0.95	2.40
$MA_{0.125}FA_{0.875}Bi_{0.375}Sb_{0.625}(I_{0.625}Se_{0.375})_3$	0.94	2.34
$MA_{0.125}FA_{0.875}Bi_{0.250}Sb_{0.750}(I_{0.625}Se_{0.375})_3$	0.93	2.19
$MA_{0.125}FA_{0.875}Bi_{0.125}Sb_{0.875}(I_{0.625}Se_{0.375})_3$	0.92	2.08
$MA_{0.125}FA_{0.875}Bi_{0.875}Cu_{0.125}(I_{0.750}Se_{0.250})_3$	**0.91**	**2.16**
$MA_{0.250}FA_{0.750}Bi_{0.875}Sb_{.125}(I_{0.625}Se_{0.375})_3$	0.91	2.55

Data collection/ organization with multicomponent perovskites

ML application on the data for E_g prediction, model selection

Data generation, T_f calculation, E_g prediction

Filtration based on crystal structure (T_f), and E_g

DFT stability calculation, further filtration

Synthesis, characterization, experimental validation

Film preparation optimization

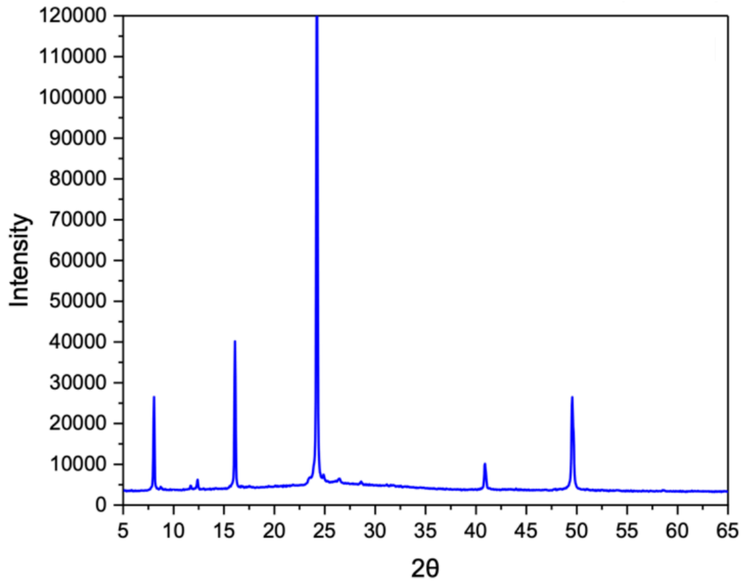
Lead free stable, efficient perovskite for solar cells

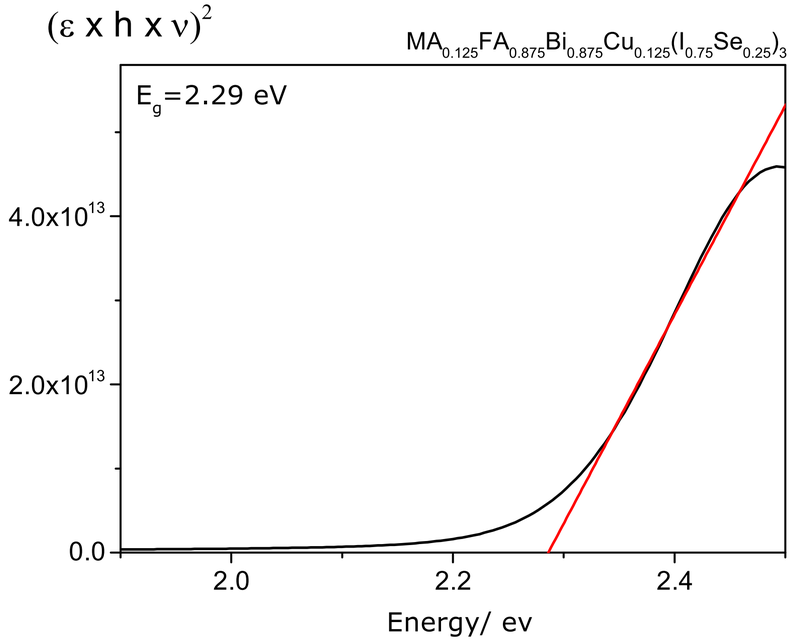
DFT and Experimental validation

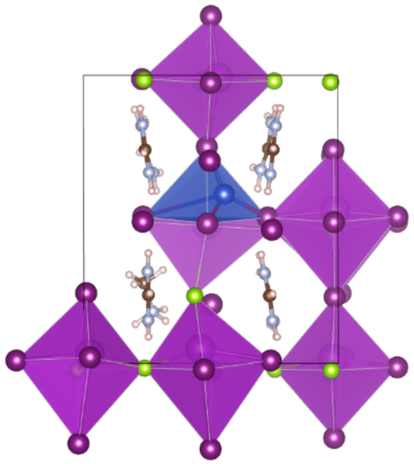
Final filter - DFT calculated stability

$MA_{0.125}FA_{0.875}Bi_{0.875}Ag_{0.125}(I_{0.750}Se_{0.250})_3 \rightarrow$ E (above hull) = 249 meV/atom (DFT), $E_g = 2.42\ ev$ (NN)

$MA_{0.125}FA_{0.875}Bi_{0.875}Cu_{0.125}(I_{0.750}Se_{0.250})_3 \rightarrow$ E (above hull) = 257 meV/atom (DFT) , $E_g = 2.16\ ev$ (NN), Experiment $\rightarrow E_g = 2.29\ ev\ (\pm 5.7\,\%)$







Data collection/ organization with multicomponent perovskites	ML application on the data for E_g prediction, model selection	Data generation, T_f calculation, E_g prediction	Filtration based on crystal structure (T_f), and E_g	DFT stability calculations, further filtration	Synthesis, characterization, experimental validation	Film preparation optimization	Lead free stable, efficient perovskite for solar cells

Further ML improvements to achieve gen. AI for perovskites

1. Collection of the data

2. Automatic organization into the table or matrix.

3. Multi-parameter prediction taking into account interconnection between the parameters.

1. Finding open source data and processing.

2. **Tokenizer**

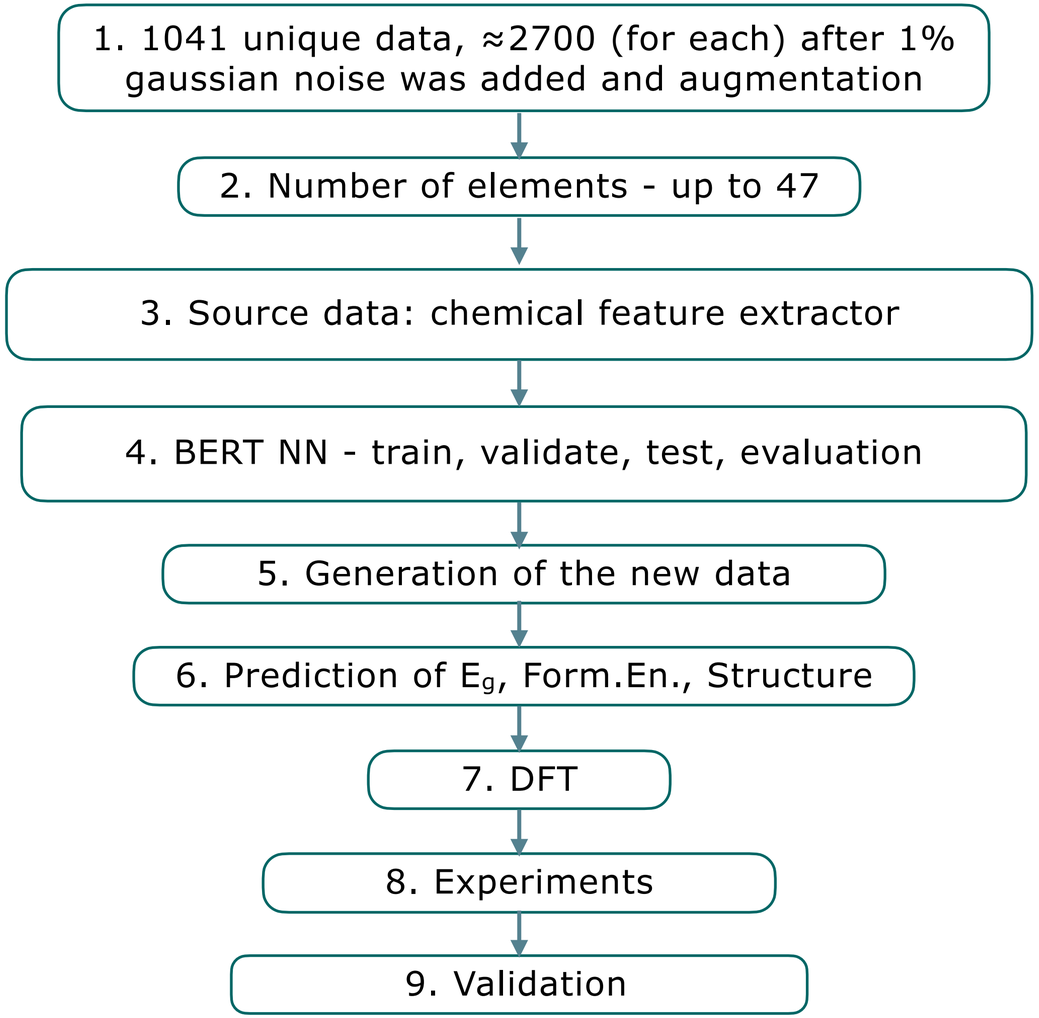
3. Bert implication (transformer and MLM).

4. Additional tools:

   A. augmentation (permutation) for imbalanced data

   B. gaussian noise 1% (exp. 7%)

   C. adding chemical or Physical meaning through important features



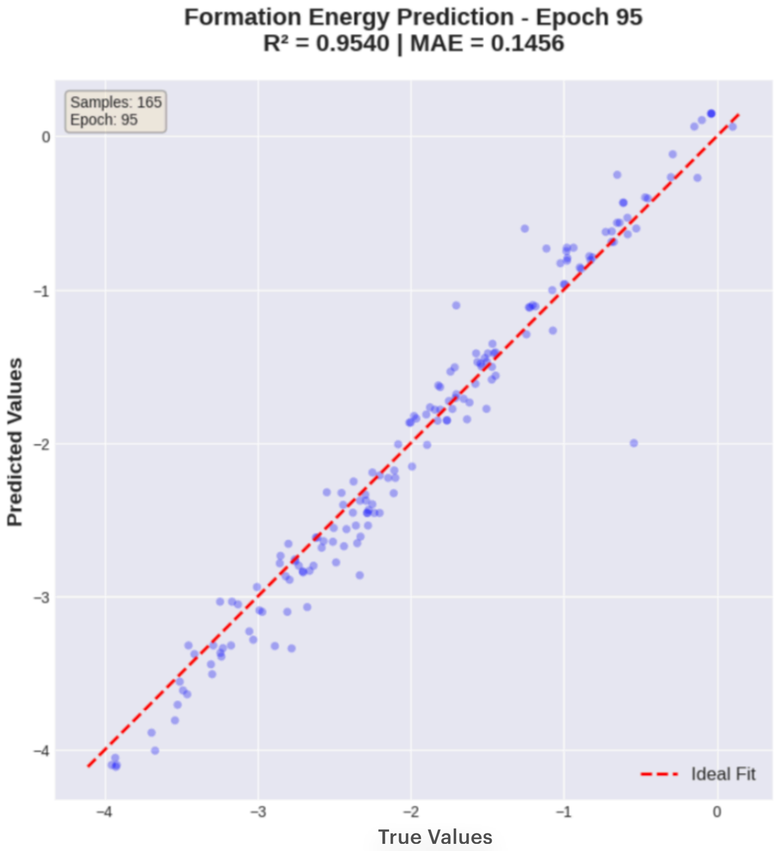
Similar approach (A, B, C) was use in PoC project from Huawei technologies, we successfully generated non organic composites meeting the expectations.

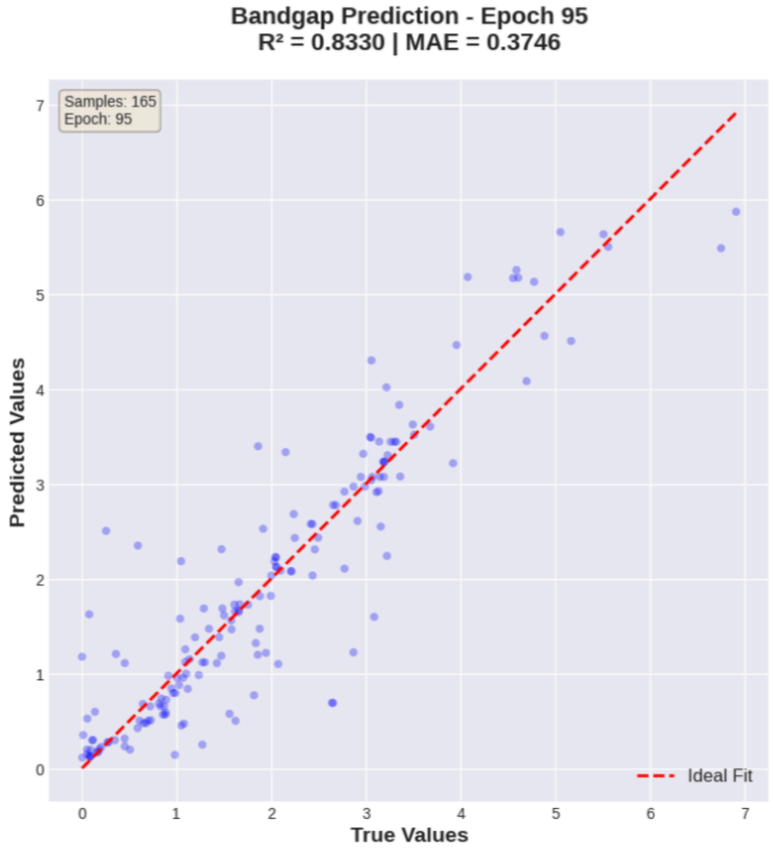
These model and tools can be used for other organic and non organic materials as well.

Next step - Generation of Perovskites by GenAI.

Data from: https://github.com/chenebuah/ML_abx3_dataset was processed

BERT results





New expanded data, automatic organizational of data

NN (BERT) simultaneous prediction of the parameters, evaluation

Build auto-encoder and include BERT NN

Generation of perovskites based on the criteria

DFT, MD validation, further filtration

Synthesis, characterization, experimental validation

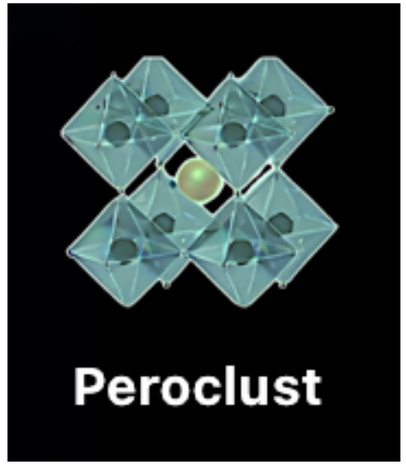
Film preparation optimization

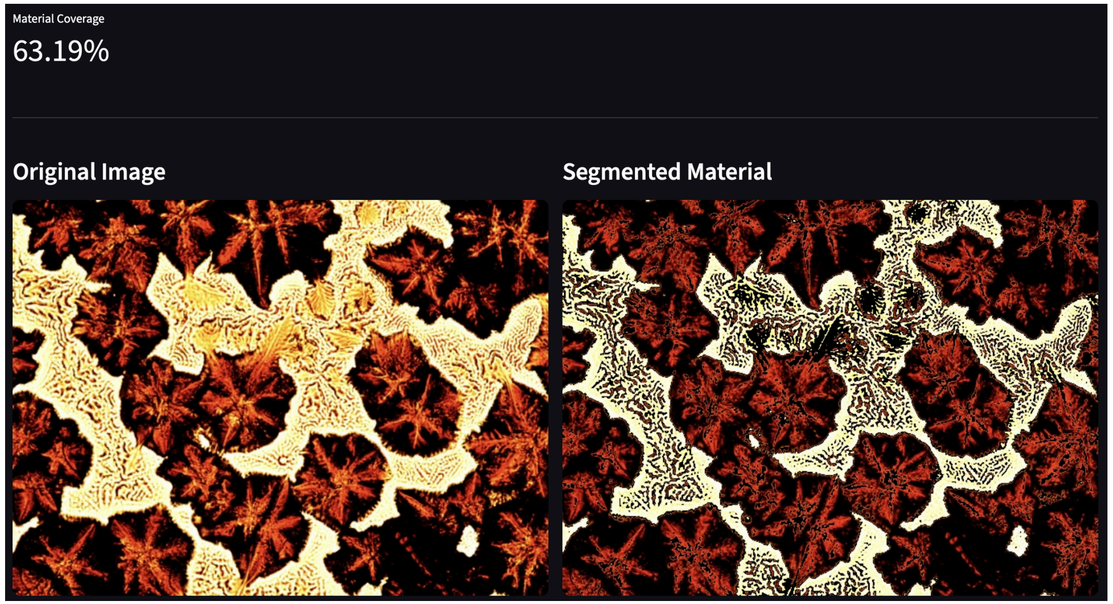
Perovskite meeting all the expectations

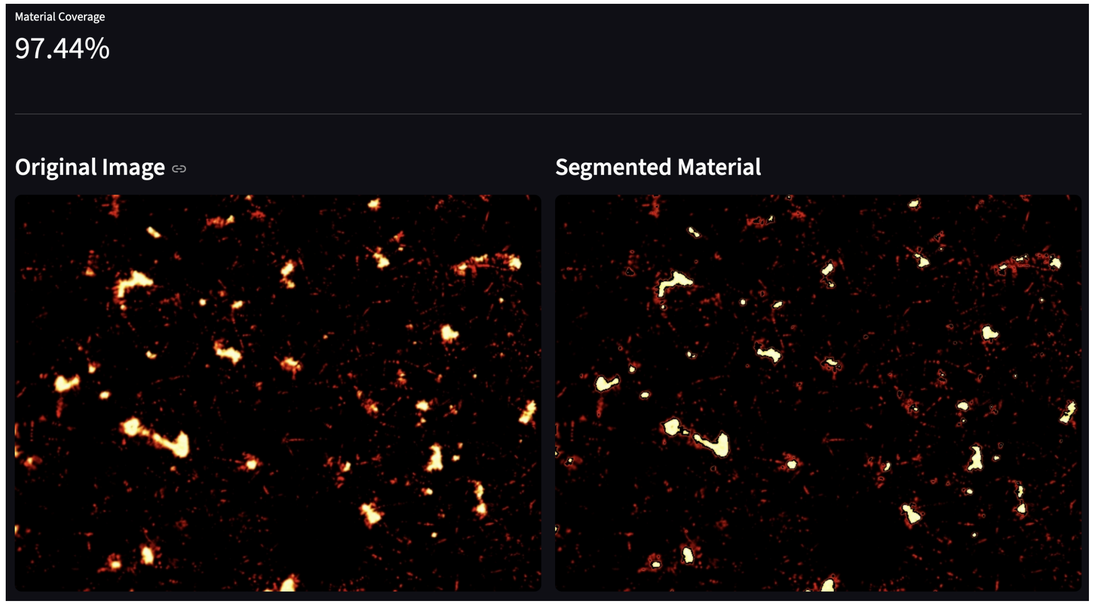
More applications …

Film preparation and characterization.

K-means clustering







State of the art optimization…

Color	sample_name	substrate_treatment	substrate_thermal_temp_c	substrate_thermal_time_min	# sc_rotation_temp	sc_step1_speed_rpm	sc_step1_head_position	# sc_step1_accel_rpm_s	sc_step1_rotation_time_s	# sc_step2_speed_rpm	sc_step2_head_position	# sc_step2_accel_rpm_s	sc_step2_rotation_time_s	processing_environment	# annealing_temp_c	annealing_duration_min	# film_coverage_pct	perovskite_solution_ul	an
FALSE	TsM 28.02.2025 2^	Standard+Pedot/PSS	100	2	115	5000	open	1500	22	7500	open	1500	45	air	150	30	72.79	200	F
FALSE	TsM 28.02.2025 3^	Standard+Pedot/PSS	100	2	115	5000	open	1500	22	7500	open	1500	45	air	150	30	75.27	200	F
FALSE	TsM 24.02.2025 4**	Standard+HCl+Pedot/PSS	100	2	115	3000	open	1500	22	7500	open	1500	45	air	150	30	78.11	200	F
FALSE	TsM 24.02.2025 5**	Standard+HCl+Pedot/PSS	100	2	115	3000	open	1500	22	7500	open	1500	45	air	150	30	84.84	200	F
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FALSE	TsM 24.02.2025 3*	Standard+HCl	100	2	115	3000	open	1500	11	7500	open	1500	30	air	150	30	83.03	200	F
FALSE	TsM 15.02.2025 1^	Standard+Pedot/PSS	100	2	115	3500	open	1500	11	5000	open	1500	30	air	150	30	76.21	200	F
FALSE	TsM 15.02.2025 2^	Standard+Pedot/PSS	100	2	115	3500	open	1500	11	5000	open	1500	30	air	150	30	91.32	200	F
FALSE	TsM 15.02.2025 3^	Standard+Pedot/PSS	100	2	115	3500	open	1500	11	5000	open	1500	30	air	150	30	80.97	200	F
FALSE	TsM 15.02.2025 4**	Standard+HCl+Pedot/PSS	100	2	115	5000	open	1500	11	7500	open	1500	30	air	150	30	88.44	200	F
FALSE	TsM 15.02.2025 5**	Standard+HCl+Pedot/PSS	100	2	115	5000	open	1500	11	7500	open	1500	30	air	150	30	82.92	200	F
FALSE	TsM 15.02.2025 6**	Standard+HCl+Pedot/PSS	100	2	115	5000	open	1500	11	7500	open	1500	30	air	150	30	83.71	200	F
FALSE	TsM 14.02.2025 1^	Standard+Pedot/PSS	100	2	115	3500	open	1500	11	5000	open	1500	30	air	150	30	78.75	200	F
FALSE	TsM 14.02.2025 2^	Standard+Pedot/PSS	100	2	115	3500	open	1500	11	5000	open	1500	30	air	150	30	79.38	200	F
FALSE	TsM 14.02.2025 3^	Standard+Pedot/PSS	100	2	115	3500	open	1500	11	5000	open	1500	30	air	150	30	79.17	200	F
FALSE	TsM 14.02.2025 4*	Standard+Pedot/PSS	100	2	115	5000	open	1500	11	7500	open	1500	30	air	150	30	80.6	200	F
FALSE	TsM 14.02.2025 5*	Standard+Pedot/PSS	100	2	115	5000	open	1500	11	7500	open	1500	30	air	150	30	78.4	200	F
FALSE	TsM 14.02.2025 6*	Standard+Pedot/PSS	100	2	115	5000	open	1500	11	7500	open	1500	30	air	150	30	74.56	200	F
FALSE	TsM 10.02.2025 1**	Standard+HCl+Pedot/PSS	100	2	115	3500	open	1000	11	5000	open	1500	30	air	150	30	66.12	200	F
FALSE	TsM 10.02.2025 2**	Standard+HCl+Pedot/PSS	100	2	115	3500	open	1000	11	5000	open	1000	30	air	150	30	77.95	200	F
FALSE	TsM 10.02.2025 1^	Standard+Pedot/PSS	100	2	115	3500	open	1000	11	5000	open	1000	30	air	150	30	76.2	200	F
FALSE	TsM 10.02.2025 2^	Standard+Pedot/PSS	100	2	115	3500	open	1000	11	5000	open	1000	30	air	150	30	82.77	200	F
FALSE	TsM 10.02.2025 3 ^	Standard+Pedot/PSS	100	2	115	3500	open	1000	11	5000	open	1000	30	air	150	30	82.31	200	F
FALSE	TsM 05.02.2025 1**	Standard+HCl+Pedot/PSS	100	2	115	3500	open	1000	11	5000	open	1000	30	air	150	30	78.35	200	F
FALSE	TsM 05.02.2025 2**	Standard+HCl+Pedot/PSS	100	2	115	3500	open	1000	11	5000	open	1000	30	air	150	30	78.79	200	F
FALSE	TsM 05.02.2025 3**	Standard+HCl+Pedot/PSS	100	2	115	3500	open	1000	11	5000	open	1000	30	air	150	30	68.38	200	F
FALSE	TsM 05.02.2025 4**	Standard+HCl+Pedot/PSS	100	2	115	3500	open	1000	11	5000	open	1000	30	air	150	30	86.2	200	F
FALSE	TsM 05.02.2025 1^	Standard+Pedot/PSS	100	2	115	3500	open	1000	11	5000	open	1000	30	air	150	30	84.72	200	F
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FALSE	TsM 18.03.2025 2^	Standard+Pedot/PSS	100	2	115	5000	open	1500	22	8500	open	1500	45	air	150	30	87.9	200	F
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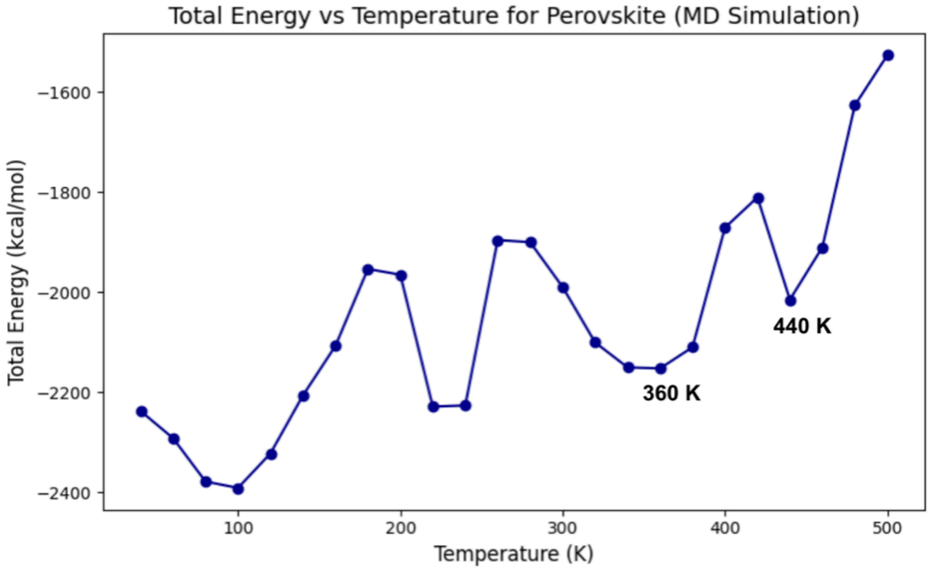
TRUE	TsM 18.03.2025 1/1^	Standard+Pedot/PSS	100	2	115	5000	open	1500	22	8500	open	1500	45	air	150	30	96.16	200	F
FALSE	TsM 18.03.2025 4**	Standard+HCl+Pedot/PSS	100	2	115	5000	open	1500	22	8500	open	1500	45	air	150	30	85.66	200	F
FALSE	TsM 18.03.2025 5**	Standard+HCl+Pedot/PSS	100	2	115	5000	open	1500	22	8500	open	1500	45	air	150	30	87.01	200	F
FALSE	TsM 18.03.2025 6**	Standard+HCl+Pedot/PSS	100	2	115	5000	open	1500	22	8500	open	1500	45	air	150	30	85.77	200	F
FALSE	TsM 21.03.2025 1^	Standard+Pedot/PSS	100	2	115	6000	open	1500	22	8500	open	1500	45	air	150	30	90.82	200	F
FALSE	TsM 21.03.2025 2^	Standard+Pedot/PSS	100	2	115	6000	open	1500	22	8500	open	1500	45	air	150	30	86.62	200	F
FALSE	TsM 21.03.2025 3^	Standard+Pedot/PSS	100	2	115	6000	open	1500	22	8500	open	1500	45	air	150	30	85.53	200	F
FALSE	TsM 21.03.2025 4*	Standard+Pedot/PSS	100	2	115	6000	open	1500	22	8500	open	1500	45	air	150	30	91.26	200	F
FALSE	TsM 21.03.2025 5**	Standard+HCl+Pedot/PSS	100	2	115	6000	open	1500	22	8500	open	1500	45	air	150	30	86.01	200	F

State of the art optimization - 2

Sample	C, g/5g	Ethylene glycol g/5g	speed, rpm	acceleration rpm/s	Duration, s	Ultrasonic bath, s	ml on glass	thickness, nm	Roughness Ra	R, kOm	UV-VIS (PEDOT:PSS)	Photos	$FAPbBr_{1.125}I_{1.875}$
1	0.0724	0.5	600	100	120	450	0.3	470	0.342	0.16			–
2	0.0724	0.5	600	100	120	450	0.3	905	0.24	0.17			–
3	0.0724	0.5	600	300	120	450	0.3	647	0.401	0.17			–
4	0.0724	0.5	600	300	120	450	0.3	450	0.2	0.11			–
5	0.0724	0.5	2000	500	30	450	0.3	360	0.258	0.36			–
6	0.0724	0.5	2000	500	30	450	0.3	238	0.221	0.39			–
7	0.0724	0.5	2000	500	30	450	0.2	292	0.382	0.46			–
8	0.0724	0.5	2000	500	30	450	0.2	464	0.312	0.52			–
9	0.069	0.5	2000	500	30	900	0.2	156	–	–			Film
10	0.069	0.5	2500	500	30	900	0.2	182	–	–			Film
11	0.069	0.5	3000	500	30	900	0.2	141	–	–			Film
12	0.069	0.5	3500	500	30	900	0.2	224	–	–			Film
13	0.069	0.5	4000	500	30	900	0.2	163	–	–			Film
14	0.069	0.5	4500	500	30	900	0.2	177	–	–			Film
15	0.069	0.5	5000	500	30	900	0.2	206	–	–			–
16	0.069	0.5	5500	500	30	900	0.2	118	–	–			–
17	0.069	0.5	5500	500	30	900	0.2	135	–	–			–
18	0.069	0.5	6000	500	30	900	0.2	110	–	–			–
19	0.069	0.5	6500	500	30	900	0.2	108	–	–			–
20	0.069	0.5	7000	500	30	900	0.2	140	–	–			–
21	0.069	0.5	7500	500	30	900	0.2	163	–	–			–
22	0.069	0.5	8000	500	30	900	0.2	120	–	–			–
23	0.0702	0.5	8000	500	30	900	0.2	72.5	0.086	3.56			–
24	0.0702	0.5	8000	500	30	900	0.2	92.5	0.278	2.51			–
25	0.0702	0.5	8000	500	30	900	0.2	92.5	0.0496	2.69			–
26	0.075	0.5	8000	500	30	900	0.2	139.5	0.0283	2.51			–
27	0.075	0.5	8000	500	30	900	0.2	123	0.085	1.95			–
28	0.075	0.5	8000	500	30	900	0.2	113.5	0.0883	2.17			–
29	0.0799	0.5	8000	500	30	900	0.2	157	0.0643	1.63			–
30	0.0799	0.5	8000	500	30	900	0.2	176.75	0.0078	1.78			–
31	0.0799	0.5	8000	500	30	900	0.2	107.25	0.089	1.72			–
32	0.0854	0.5	8000	500	30	900	0.2	156.75	0.0436	1.69			–
33	0.0854	0.5	8000	500	30	900	0.2	211.75	0.0463	1.52			–
34	0.0854	0.5	8000	500	30	900	0.2	179	0.183	1.29			–
35	0.0903	0.5	8000	500	30	900	0.2	145.25	0.078	1.37			–
36	0.0903	0.5	8000	500	30	900	0.2	227	0.081	1.34			–
37	0.0903	0.5	8000	500	30	900	0.2	179.25	0.067	1.35			–
38	0.095	0.5	8000	500	30	900	0.2	138.5	0.066	1.17			–
39	0.095	0.5	8000	500	30	900	0.2	161	0.056	1.94			–
40	0.095	0.5	8000	500	30	900	0.2	186	0.102	01.01			–
41	0.1	0.5	8000	500	30	900	0.2	251.75	0.101	0.84			–
42	0.1	0.5	8000	500	30	900	0.2	199.5	0.182	0.87			–
43	0.1	0.5	8000	500	30	900	0.2	158.75	0.138	0.73			–
44	0.1053	0.5	8000	500	30	900	0.2	170.25	0.102	0.84			–
45	0.1053	0.5	8000	500	30	900	0.2	161	0.146	0.86			–
46	0.1053	0.5	8000	500	30	900	0.2	208.75	0.140	0.84			–
47	0.1	0	8000	500	30	0	0.2	189	0.194	–			–

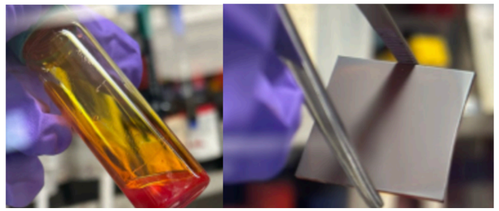
Sample	Samples of PEDOT	C g/ml	Speed, rpm		Acceleration rpm/s		Duration, s	Thickness, nm	Roughness Ra	Photos under microscope and coverage/ $FAPbBr_{1.125}I_{1.875}$	Bandgap, EV
			step 1	step 2	step 1	step 2	step 1				
1	9	0.8476	6500	9500	1500	1500	22	102	–		
2	10	0.8477	6500	9500	1500	1500	22	139	–		
3	11	0.8478	6500	9500	1500	1500	22	172	–		
4	12	0.8479	6500	9500	1500	1500	22	146	–		
5	13	0.8480	6500	9500	1500	1500	22	92	–		
6	14	0.8481	6500	9500	1500	1500	22	74	–		
7	56	0.8487	5000	9500	1500	2000	22	462	0.424		
8	57	0.8488	5000	9500	1500	2000	22	282.25	0.551		
9	58	0.8489	5000	9500	1500	2000	22	253.25	0.323		
10	74	0.8490	5000	9500	1500	2000	22	437.5	0.345		
11	75	0.8491	5000	9500	1500	2000	22	481	0.353		
12	76	0.8492	5000	9500	1500	2000	22	430.75	0.332		
13	77	0.8493	5000	9500	1500	2000	22	367	0.584		
14	78	0.8494	5000	9500	1500	2000	22	283.5	0.393		
15	79	0.8495	5000	9500	1500	2000	22	582.25	0.596		

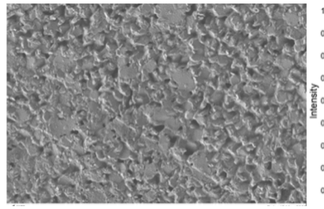


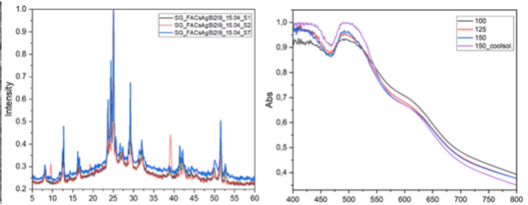
Perovskites synthesized by our chemists

1. $CsPbBr_2I$
2. $CsPbBrI_2$
3. $FAPbBr_{1.125}I_{1.875}$
4. $FACsAgBi_2I_9$
5. $DMACsAgBi_2I_9$
6. $MA_{0.125}FA_{0.875}Bi_{0.875}Cu_{0.125}I_{0.750}Se_{0.250}$
7. $MA_{0.125}FA_{0.875}Bi_{0.875}Ag_{0.125}I_{0.750}Se_{0.250}$

+ precursors







Our next and ongoing steps

1. Cell preparation - direct and inverted structure.

2. Optimization for Lead free perovskites' synthesis and film preparation.

3. New NN results using wider range of elements, predicting 3 parameters simultaneously and filtering for solar cell and display applications.

4. DFT confirmation of results, structure and stability calculations.

5. MD simulations - for time, temperature, environmental stability.

Devices obtained in 2025

1. Nitrogen Generator - Minnuo MNPN 3/99.999

2. Vacuum Ball Milling Device - XQM-2A

Publications

1. Sona Grigoryan, Nane Petrosyan, Gurgen Kolotyan, Arpine Kozmanyan, Varazdat Avetisyan, Hayk Zakaryan, Michael J. Schöning, Arevik Asatryan, Hayk Khachatryan. “Accelerated composition optimization of hybrid perovskites via data-driven materials design, DFT calculations and synthesis”. Materials & Design, 260, 114902, 2025. DOI: 10.1016/j.matdes.2025.114902 (Q1, IF=7.1)

2. Tamar Danielyan, Arevik Asatryan, Arsen Sahakyan, and Hayk Khachatryan. Enhancing perovskite solar cell efficiency and stability through architectural modifications and additives. Journal of Power Sources 630, 235995, 2025. DOI: 10.1016/j.jpowsour.2024.235995 (Q1, IF=7.1)

3. Sadegh Kaviani. Covalent organic framework-based solid polymer electrolytes for metal-ion batteries: pioneering the future of DFT, MD, and ML techniques. Energy Storage Materials 82, 104671, 2025. DOI: 10.1016/j.ensm.2025.104671. (Q1, IF=20.2)

4. Sadegh Kaviani. Molecular dynamics and machine learning framework for predicting ion transport and mechanical properties of ionic liquid@polyvinylidene fluoride gel polymer electrolyte" Journal of Industrial and Engineering Chemistry 2025. DOI: https://doi.org/10.1016/j.jiec.2025.11.034. (In Press, Q1, IF=5.9)

5. Irina I. Piyanzina, Regina M. Burganova, Sadegh Kaviani, Oleg V. Nedopekin and Hayk Zakaryan. “A DFT study on an 18-crown-6-like-N8 structure as a material for metal ion storage: stability and performance”. Sustainable Energy Fuels 18, 2025. DOI: 10.1039/D5SE00333D (Q1, IF=4.1)

6. Shamsieva Aigul, Alexander Evseev, Sadegh Kaviani, Oleg V. Nedopekin, Hayk Zakaryan, and Irina I. Piyanzina. "DFT analysis of furan-based covalent organic framework as electrode materials for lithium and calcium ion batteries." Computational and Theoretical Chemistry 1253, 115445, 2025. DOI: 10.1016/j.comptc.2025.115445 (Q3, IF=2.8)

7. Левченко Д.С., Никогосян М.Г., Асатрян. А.В. “Дифференциальные кривые плавления для сгенерированных случайных и реальных последовательностей в ДНК.” Вестник РАУ 082, 148-155, 2025. https://science.rau.am/uploads/documents/1751527835.pdf

+ three papers submitted (two of them are under review).
+ two drafts are on last stages.

Conferences

1. 7th Edition of Advanced Materials Science World Congress - Gurgen Kolotyan, Sona Grigoryan, Nane Petrosyan, Michael J. Schöning, Hayk Zakaryan, Hayk Khachatryan, Arevik Asatryan - Optical Properties and Band Gap Analysis of Perovskite Thin Films (London, United Kingdom, Oral presentation: Arevik Asatryan).

2. ICMSE 2025: 19. International Conference on Materials Science and Engineering - Sona Grigoryan, Mikael Ghevondyan, Michael Josef Schöning, Hayk Khachatryan, Arevik Asatryan - Optimization Strategy of Effective Perovskite thin films (Florence, Italy, Oral presentation: Sona Grigoryan - won the **best presentation prize**).

3. AI4X 2025 International Conference - Gurgen Kolotyan, Hayk Khachatryan, , Arevik Asatryan - Finding Perovskite Composites With Preferable Features: Simple ML algorithms (Singapore, Oral presentation: Gurgen Kolotyan).

4. Renewableeeng-2025 - Sona Grigoryan, Hayk Khachatryan, Arevik Asatryan - Enhancing the Morphology of Cs-Based Perovskite Thin Films Through Material Engineering (Barcelona, Spain, Oral presentation: Sona Grigoryan)

5. Renewableeeng-2025 - Nane Petrosyan, Hayk Zakaryan, Hayk Khachatryan, Arevik Asatryan - Influence of Atom Positioning on Stability of Perovskites (Barcelona, Spain, Oral presentation: Nane Petrosyan).

Three proceedings.

Other Visits

1. PI of the project Hayk Khachatryan visited FMG, IChPh during 23.06.-23.07.2026.

2. Sona Grigoryan visited Tampere University (Tampere, Finland) and National Institute of Chemistry (Ljubljana, Slovenia) for a joint research - synthesis of perovskites for solar cell applications, synthesis and utilization of MOF systems for stability of Perovskites (24-YSIP-009, 22RL-012).

Deepening international collaborations

1. MoU with INB - 28.11.2025.

2. Preparing European project with Prof. Schöning (INB).

3. Submitted the second manuscript with INB team.

5. Agreed with Prof. Paola Vivo for Sona’s next visit for solar cell device preparation in Tampere University.

6. Continue the collaboration with National Institute of Chemistry (Slovenia).

Deepening local collaborations

1. Laboratory of Macrokinetics of Solid State Reactions applied for Horizon project and FMG is participating in the project (04.2026).

2. Continue the collaboration with YSU.

3. A. Alikhanyan National Laboratory.

Deepening inter-institute collaborations

1. 3D Printing Research Laboratory

2. Liquid Crystalline Nanosystems Research Group

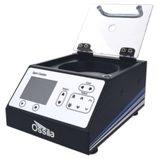
3. Laboratory of Macrokinetics of Solid State Reactions

4. Laboratory of Catalysis

New projects and dissemination

1. Postdoctoral project by Dr. Sadegh Kaviani.

2. Equipment grant (20 000 000 amd).



3. Huawei technologies co. ltd - 12400 Euro

Huawei Technologies Oy (Finland) Co. Ltd
Läkkisepäntie 23, 00620 Helsinki, Finland
Website: www.huawei.com

Confidential

Confirmation of Successful Project Completion

To Whom It May Concern,

This is to formally confirm that **Huawei Technologies Oy (Finland R&D Center)** and the **Institute of Chemical Physics, Armenia,** have successfully completed the Proof-of-Concept (PoC) project entitled:

"AI Model Development for Optimization of the LM Composition."

Throughout the course of this collaboration, the **Functional Materials Laboratory** of the Institute of Chemical Physics provided all required deliverables in a timely and professional manner. The team was able to develop , train, and apply a machine learning model capable of predicting liquid metal (LM) compositions that met the project's technical requirements.

We highly value the expertise and contributions of the Institute of Chemical Physics, which were essential to the success of this PoC project.

We look forward to potential opportunities for further collaboration in the future.

For further information, you may contact:

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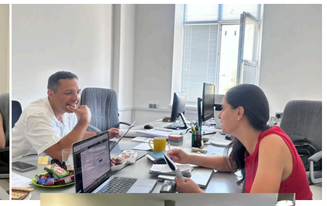
Head of Thermal Management Group
Huawei Technologies Oy (Finland) Co. Ltd
Hayk.khachatryan@huawei.com
+358 44 706 25 96

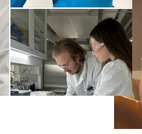
22.09.2025

4. Participation in EIF-PMI organized forum in Tsaghkadzor.

5. Dissemination through various tools - Publications, social network, Science week, receiving students for tours, conferences, etc.

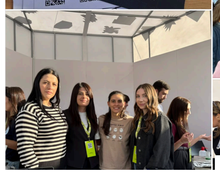
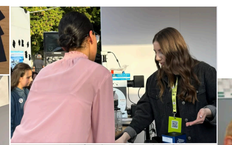
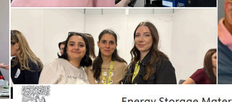











Energy Storage Materials
Available online 8 October 2025, 104671
In Press, Journal Pre-proof What's this?

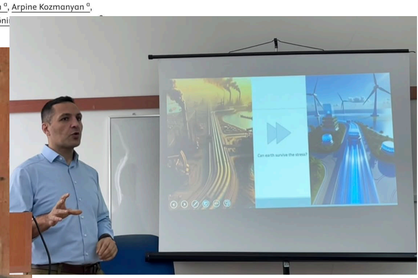
Covalent organic framework-based solid polymer electrolytes for metal-ion batteries: pioneering the future of DFT, MD, and ML techniques

Sadegh Kaviani
A.B. Nalbandyan Institute of Chemical Physics NAS RA, 5/2 P. Sevak Street, 0014, Yerevan,

Materials & Design
Available online 17 October 2025, 114902
In Press, Journal Pre-proof What's this?

Accelerated composition optimization of hybrid perovskites via data-driven materials design, DFT calculations and synthesis

…na Grigoryan[a], Nane Petrosyan[a,b], Gurgen Kolotyan[a], Arpine Kozmanyan[a], …razdat Avetisyan[a], Hayk Zakaryan[b], Michael J. Schöni…
…yk Khachatryan[a]

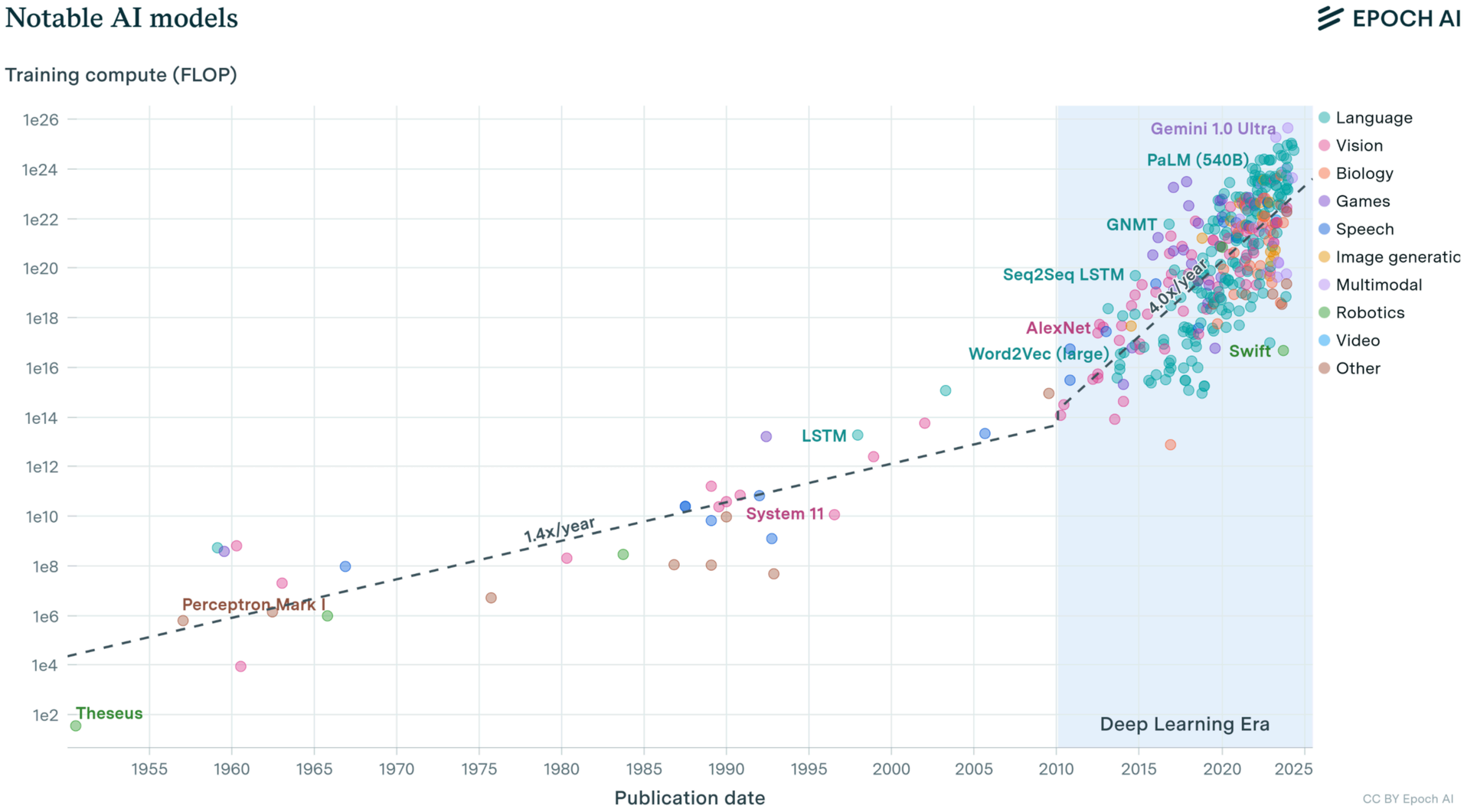

Thank you

ML selected list of the compositions

- Laboratory ready -> synthesis -> characterization (band gap calculation) -> another cycle of ML training with the new data.

Cs	MA	FA	Pb	Cl	Br	I
xA	yA	zA	B	xC	yC	zC
0.1	0.1	0.8	1	0	0	1
0.1	0.1	0.8	1	0.2	0.7	0.1
0.1	0.1	0.8	1	0.7	0.1	0.2
0.1	0.2	0.7	1	0	0	1
0.1	0.2	0.7	1	0.2	0.7	0.1
0.1	0.2	0.7	1	0.7	0.1	0.2
0.2	0.1	0.7	1	0	0	1
0.2	0.1	0.7	1	0.2	0.7	0.1
0.2	0.1	0.7	1	0.7	0.1	0.2
0.2	0.2	0.6	1	0	0	1
0.2	0.2	0.6	1	0.2	0.7	0.1
0.2	0.2	0.6	1	0.7	0.1	0.2
0.3	0.1	0.6	1	0	0	1
0.3	0.1	0.6	1	0.2	0.7	0.1
0.3	0.1	0.6	1	0.7	0.1	0.2
0.1	0.3	0.6	1	0	0	1
0.1	0.3	0.6	1	0.2	0.7	0.1
0.1	0.3	0.6	1	0.7	0.1	0.2
0.2	0	0.8	1	0	0	1
0.2	0	0.8	1	0.2	0.7	0.1
0.2	0	0.8	1	0.7	0.1	0.2
0.3	0	0.7	1	0	0	1
0.3	0	0.7	1	0.2	0.7	0.1
0.3	0	0.7	1	0.7	0.1	0.2
0	0.4	0.6	1	0	0	1
0	0.4	0.6	1	0.2	0.7	0.1
0	0.4	0.6	1	0.7	0.1	0.2

AI evolution



J. Sevilla, L. Heim, A. Ho, T. Besiroglu, M. Hobbhahn and P. Villalobos, "Compute Trends Across Three Eras of Machine Learning," 2022 International Joint Conference on Neural Networks (IJCNN), Padua, Italy, 2022, pp. 1-8, doi: 10.1109/IJCNN55064.2022.9891914.

Source: https://epoch.ai/blog/compute-trends

1. We chose $FAPb(Br_{0.375}I_{0.625})_3$ composite based on its Goldschmidt's tolerance factor value ($t = \frac{r_A + r_x}{\sqrt{2}\,(r_B + r_x)}$), band gap energy, good agreement of its value within different models and with DFT results, and presence of precursors in our laboratory.

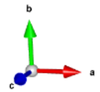
2. For this composite the further investigation was carried out.

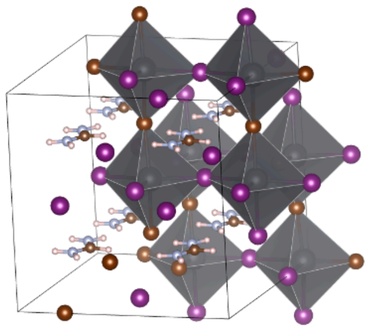
$FAPb(Br_{0.375}I_{0.625})_3$ Convex hull Results

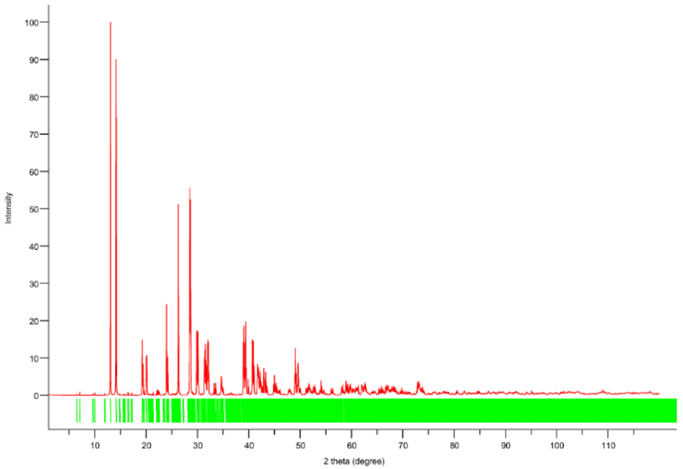
Without cell shape relaxation
E_above_hull ≈ 0.2457 ev

With cell shape relaxation
E_above_hull ≈ 0.2441 ev

FaPb($I_{0.625}Br_{0.375}$)$_3$: XRD Data From Calculations







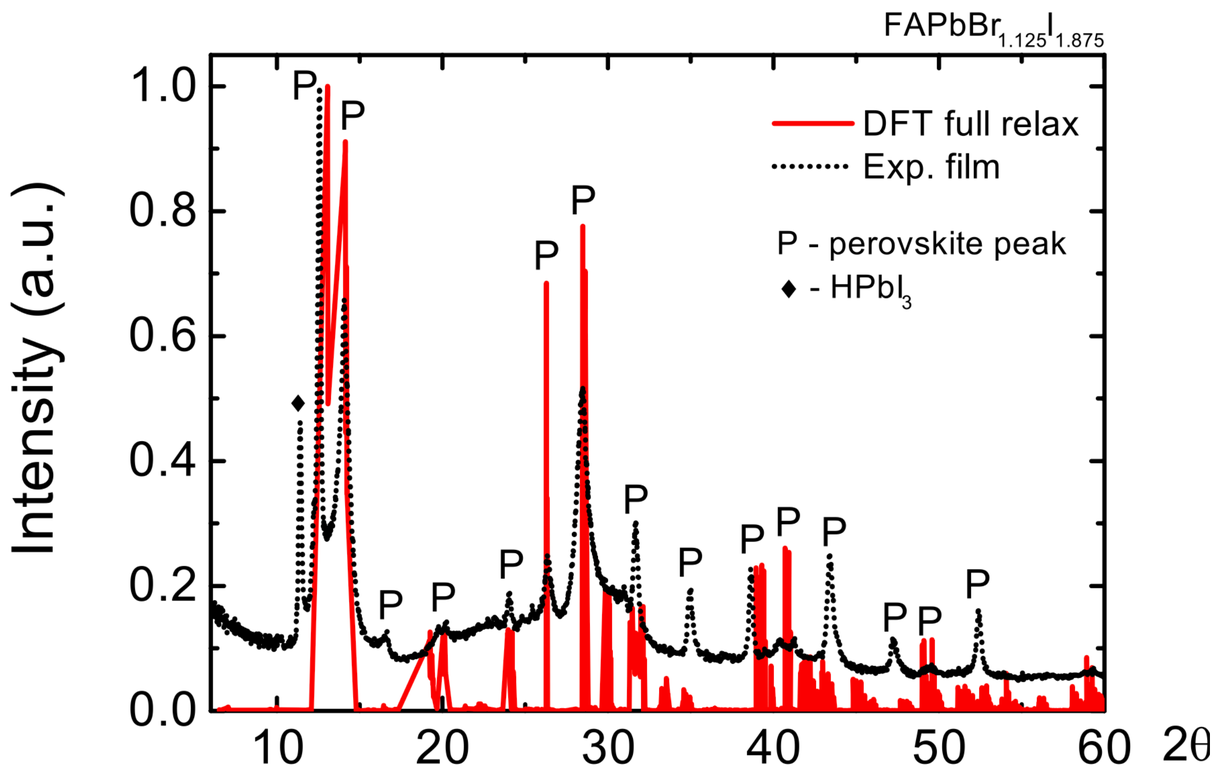
$FAPb(Br_{0.375}I_{0.625})_3$ energies per atoms depending on atom position

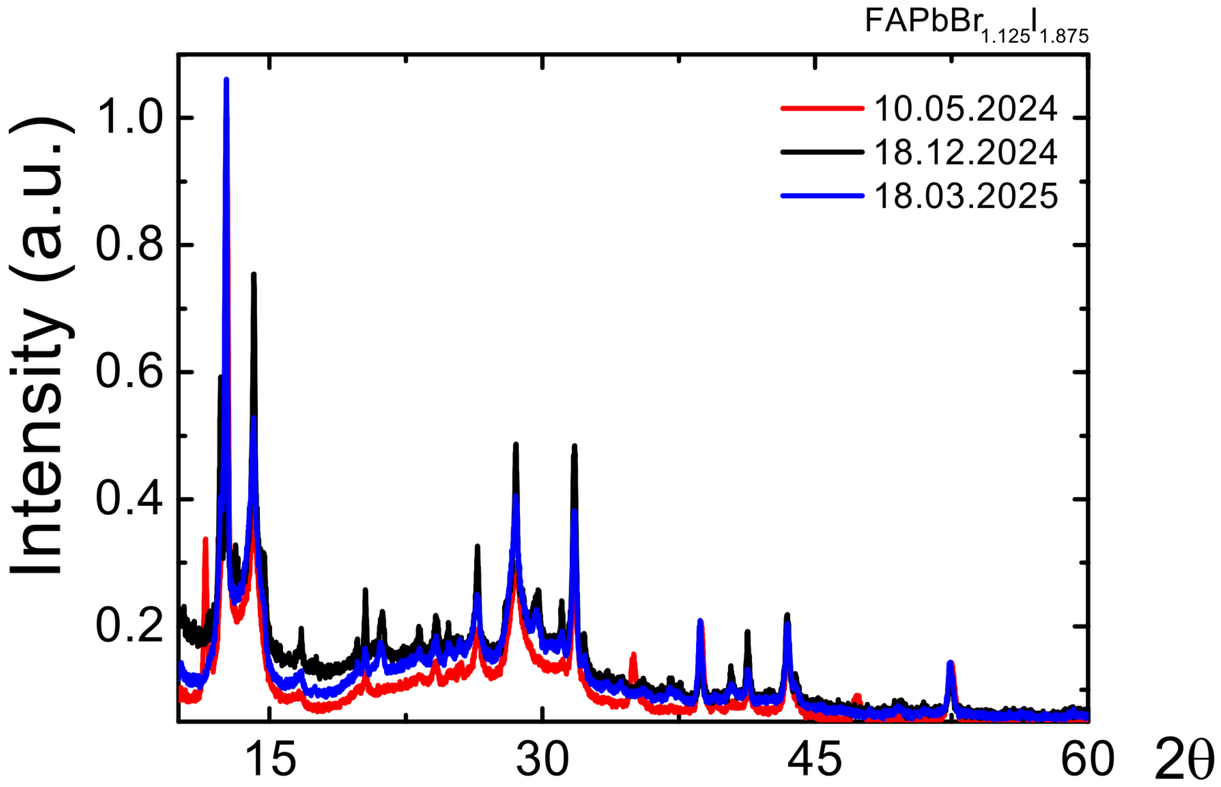
$FaPb(I_{0.625}Br_{0.375})_3$ Calculations for Novel 10 Materials

Energy comparison

Structure_number	Total_energy	Total_energy_per_atom
Structure_1	-444.4995966	-4.630204132
Structure_2	-444.4706286	-4.629902381
Structure_3	-445.2771196	-4.638303329
Structure_4	-444.6006257	-4.631256517
Structure_5	-444.4608491	-4.629800512
Structure_6	-444.8655887	-4.634016549
Structure_7	-444.1200095	-4.626250099
Structure_8	-444.5813482	-4.631055711
Structure_9	-444.1950171	-4.627031429
Structure_10	-444.1676187	-4.626746028

XRD results' from DFT: $FAPb(Br_{0.375}I_{0.625})_3$ and experimental films, stability after 7 months



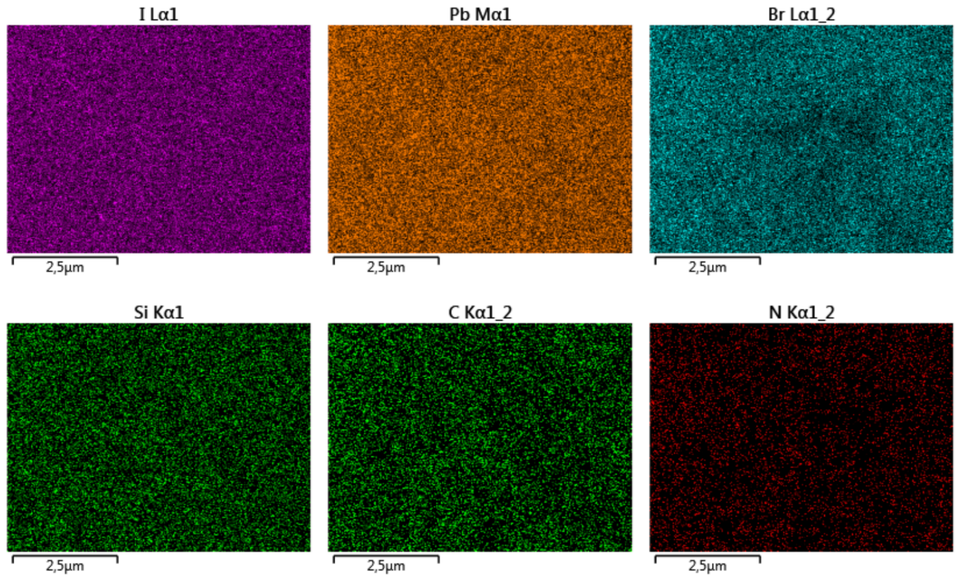


National Academy of Sciences
A.B. Nalbandyan
Institute of Chemical Physics

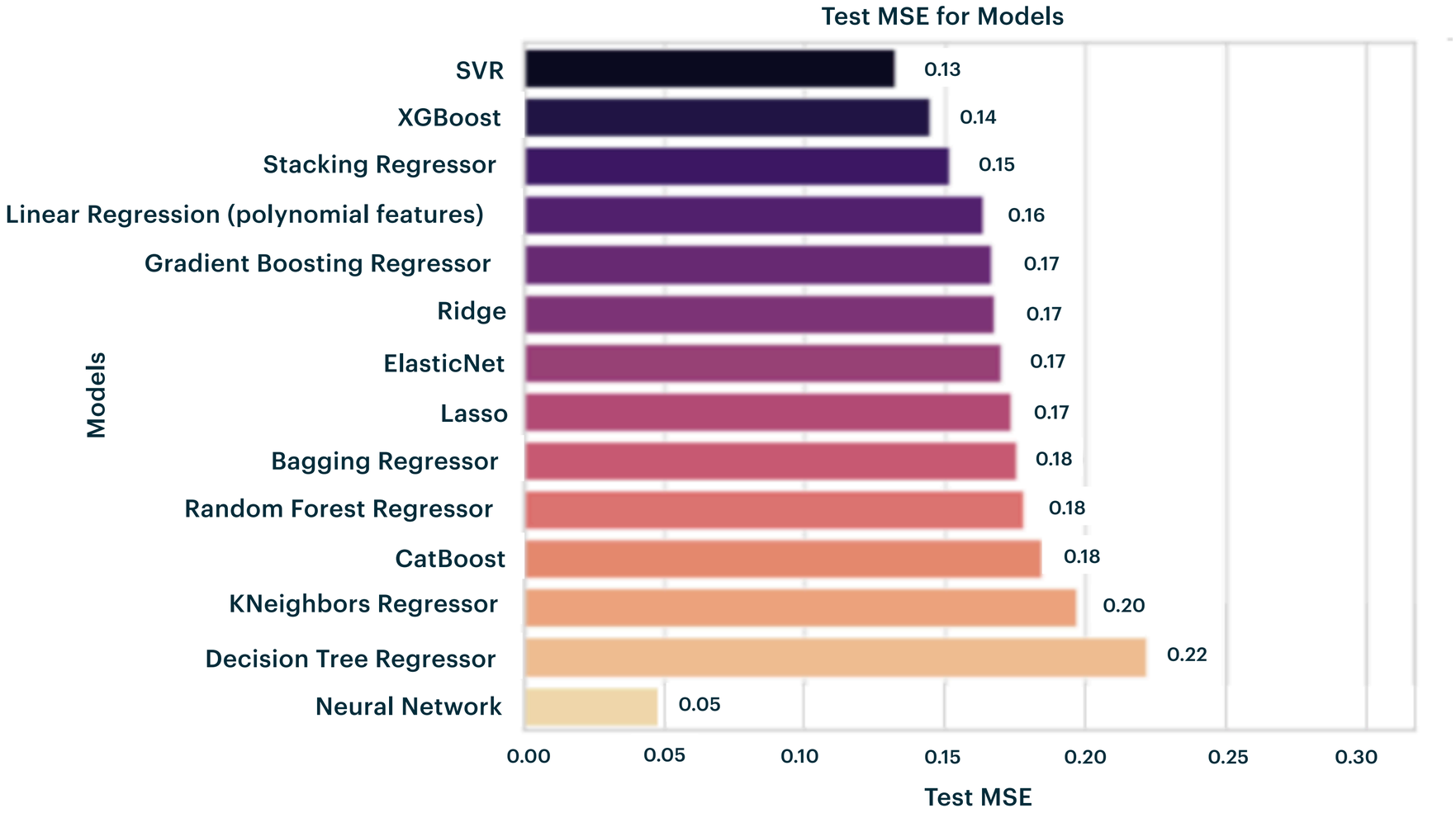
$FAPb(Br_{0.375}I_{0.625})_3$ sample 10

INB

All the elements are homogeneously spread in the sample.



Complicated problems - deep learning



Data Sources for unique 1041 perovskites

Database	Concise summary	URL
Materials Project	Information on the characteristics of natural and fictitious materials	https://materialsproject.org
Crystal Structure for Inorganic compounds	Experimentally derived crystal structure characterization data	https://icsd.fiz-karlsruhe.de
Structural	The Cambridge Crystallographic Data Centre's library of tiny molecule and metal-organic molecular crystallographic structures is developed on XRD and neutron diffraction investigations.	https://www.ccdc.cam.ac.UK/
Aflow - Automatic-FLOW for the Discovery of Materials	A data of inorganic material properties and structures derived from high-throughput ab initio calculations	http://www.aflowlib.org/
Crystallography	Information about the structures of minerals, metal-organic complexes, and organic molecules	http://cod.ensicaen.fr/
Quantum Materials	Data from theoretical simulation calculations, mainly for fictitious materials	https://www.oqmd.org/
Materials	The most extensive material data resource in the world. A distinct, superior numerical data	https://materials.springer.com/
GDB	Data of fictitious tiny organic molecules	https://gdb.unibe.ch/downloads/
ZINC	Two- and three-dimensional organic compounds that are obtainable commercially	https://zinc15.docking.org/
Material	Data of topological materials	http://materiae.iphy.ac.cn
Materials Cloud	Information from structural calculations of potential 2-D materials	https://www.materialscloud.org
Materials Database Platform for Data-Science	Peer-reviewed phase diagram, physical properties, or crystal structure	https://mpds.io
Perovskite Solar Cells	Device structure with output solar cell parameters	http://perovskite.info/perovSearch
HybriD^3 materials	Information about lattice parameters and crystal system of material	https://materials.hybrid3.duke.edu/
Materials Zone platform	The database covered almost 42 500 device data on the basis of cell architecture, deposition procedure, stability protocols, etc.	https://app.materials.zone/signin
Refractive Index	Information about refractive index, extinction coefficient, dielectric constant, absorption coefficient, and transmittance of materials	https://refractiveindex.info/
Crystallography	Lattice system, interaxial angles, edge lengths, space group, and other crystallographic information of material	http://www.crystallography.net/cod/
International Center for Diffraction Data	Collection of powder diffraction data to identify materials	https://www.icdd.com/

1. 110 collected by FMG
https://www.sciencedirect.com/science/article/pii/S026412752501322X#fig0015

2. 320 collected and processed by FMG
Will be available, when the article is published

1. Firstly, the XRD spectra of synthesized $FAPb(Br_{0.375}I_{0.625})_3$ were compared with XRD spectra of its precursors to insure that, new material has been obtained.

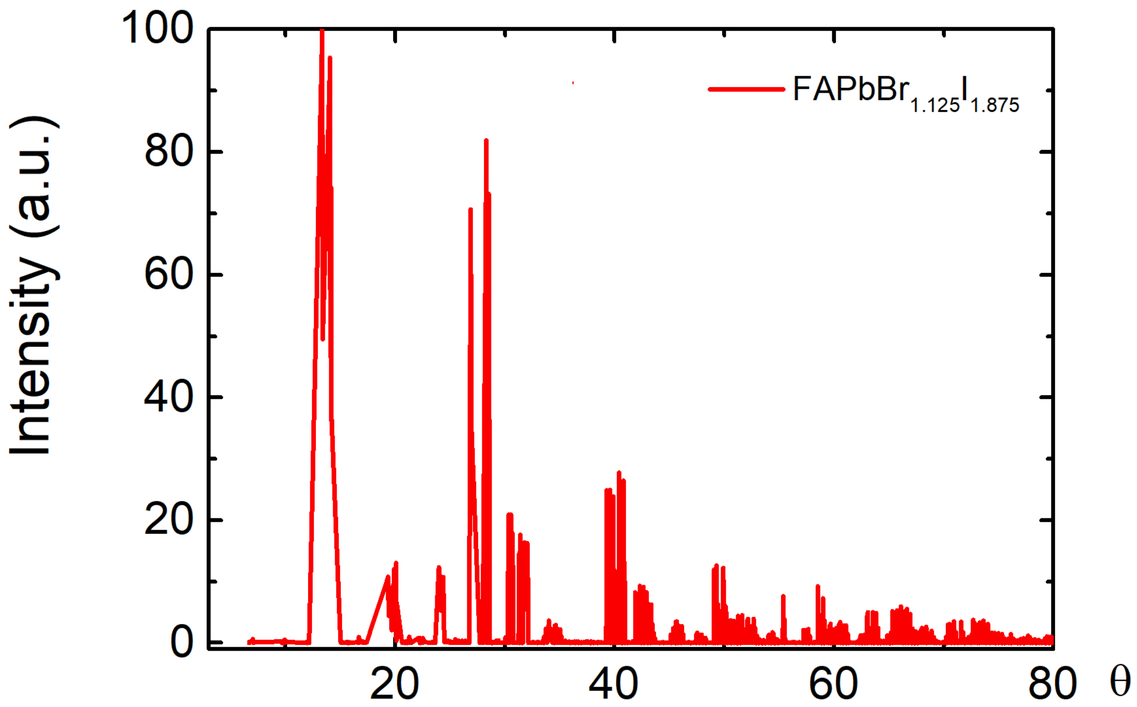
2. Then, the XRD results from DFT calculations has been compared to the XRD spectra of synthesized $FAPb(Br_{0.375}I_{0.625})_3$.

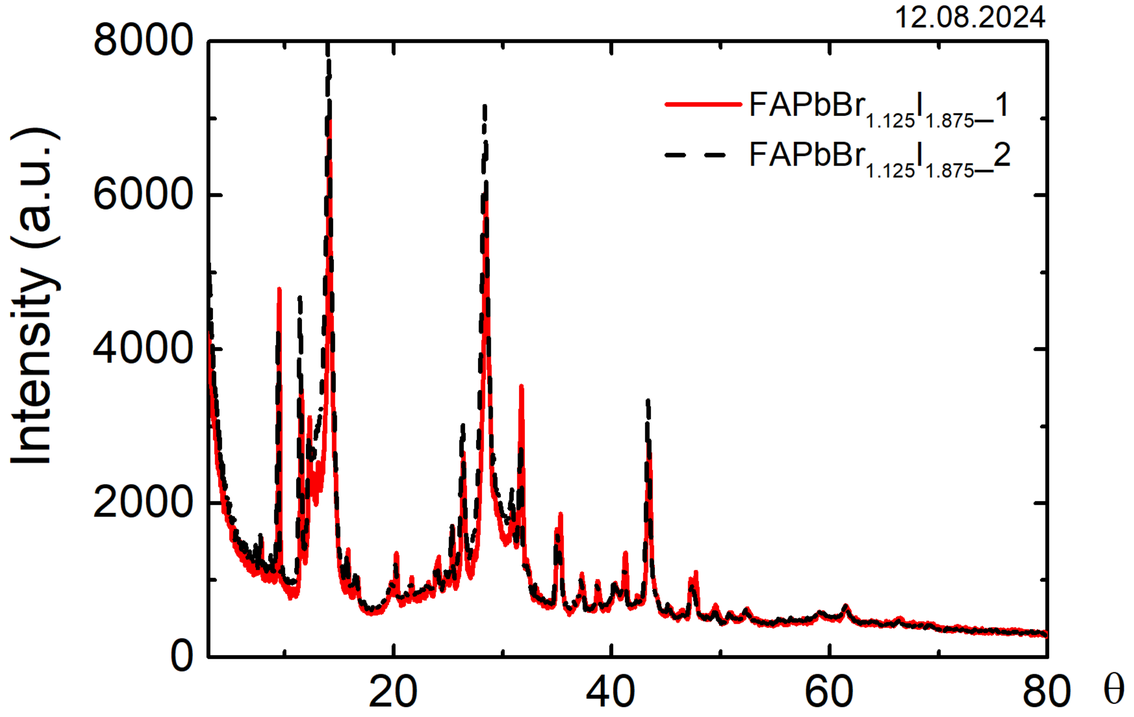
1. The comparison with the precursors show that only several small peaks of obtained perovskites are in agreement with precursors, which means, that small amount of precursors are still in the final solution of perovskite.
2. The main high peaks indicate phase, different from all the precursors.

In all the comparisons shift $\leq 0.04^0$ is considered as the same peak.

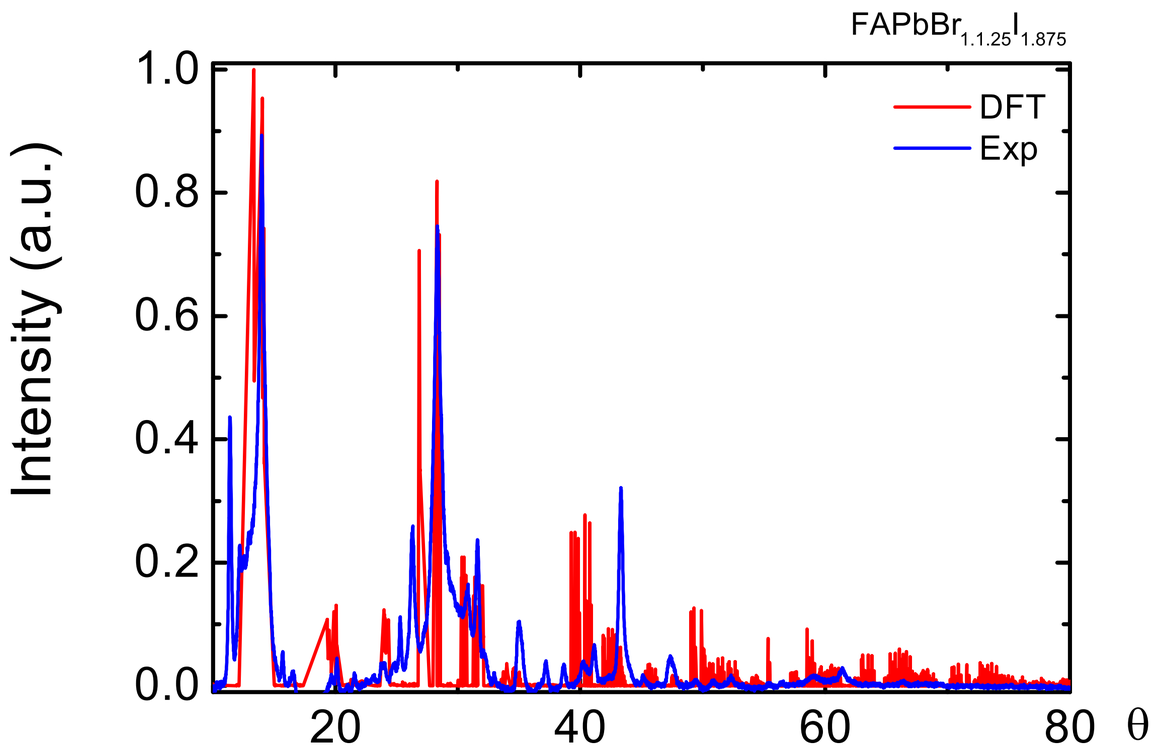
Thus the comparison with the DFT results follows:

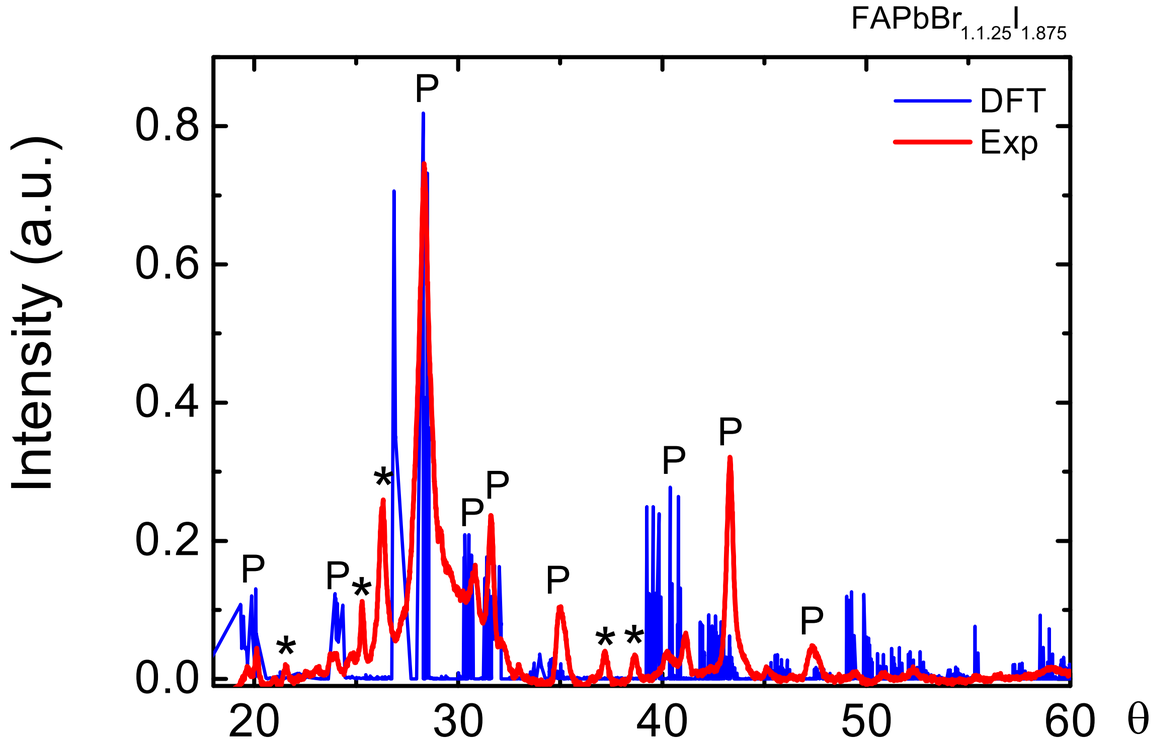
XRD results' from DFT: $FAPb(Br_{0.375}I_{0.625})_3$ cubic sample and 2 experimental films 12.08.2024





XRD results' from DFT: $FAPb(Br_{0.375}I_{0.625})_3$ cubic sample and experimental 12.08.2024

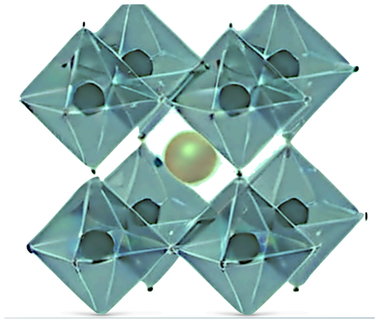




From the comparison of DFT and experimental results it is clear, that main peaks are in agreement, however, some of them are better expressed on experimental spectrum, some: on DFT spectrum.

Thus, we were able to obtain the selected perovskite in ambient conditions, which is relatively stable (gathered similar results during 1.5 month period, while keeping in the air, under the daylight).

The solution contains very small amount precursors, thus on the experimental XRD spectra some additional peaks of precursors are present, and some perovskite original peaks are smaller.



UV-VIS SPECTROSCOPY RESULTS

DFT results

DFT calculations showed that $E_g = 1.69$ ev for $FAPb(Br_{0.375}I_{0.625})_3$.

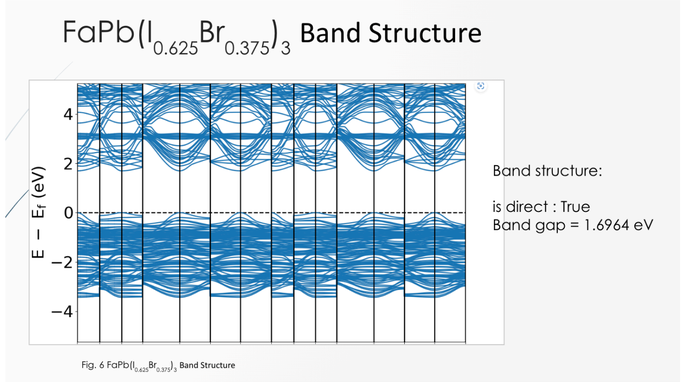


Fig. 6 $FaPb(I_{0.625}Br_{0.375})_3$ Band Structure

To make the results more precise, corrections through adding potentials for selected elements were applied. In case of Br and I there was no difference. While the energy was slightly increased when the potential was applied for Pb. For 20 ev potential correction, the band gap energy was calculated $E_g = 1.73$ ev.

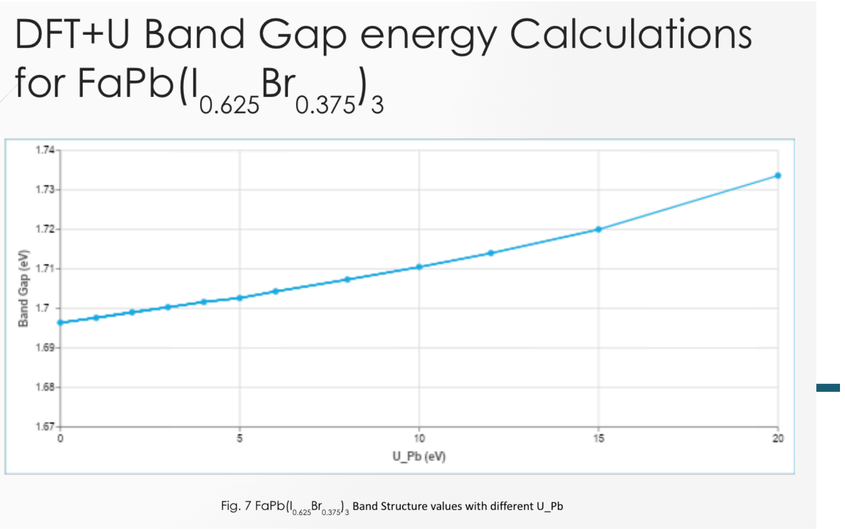


Fig. 7 $FaPb(I_{0.625}Br_{0.375})_3$ Band Structure values with different U_Pb

UV-Vis results and band gap energy from experiment: $FAPb(Br_{0.375}I_{0.625})_3$

UV-Vis spectra were used to draw Tauc plot and calculate band gap energies.

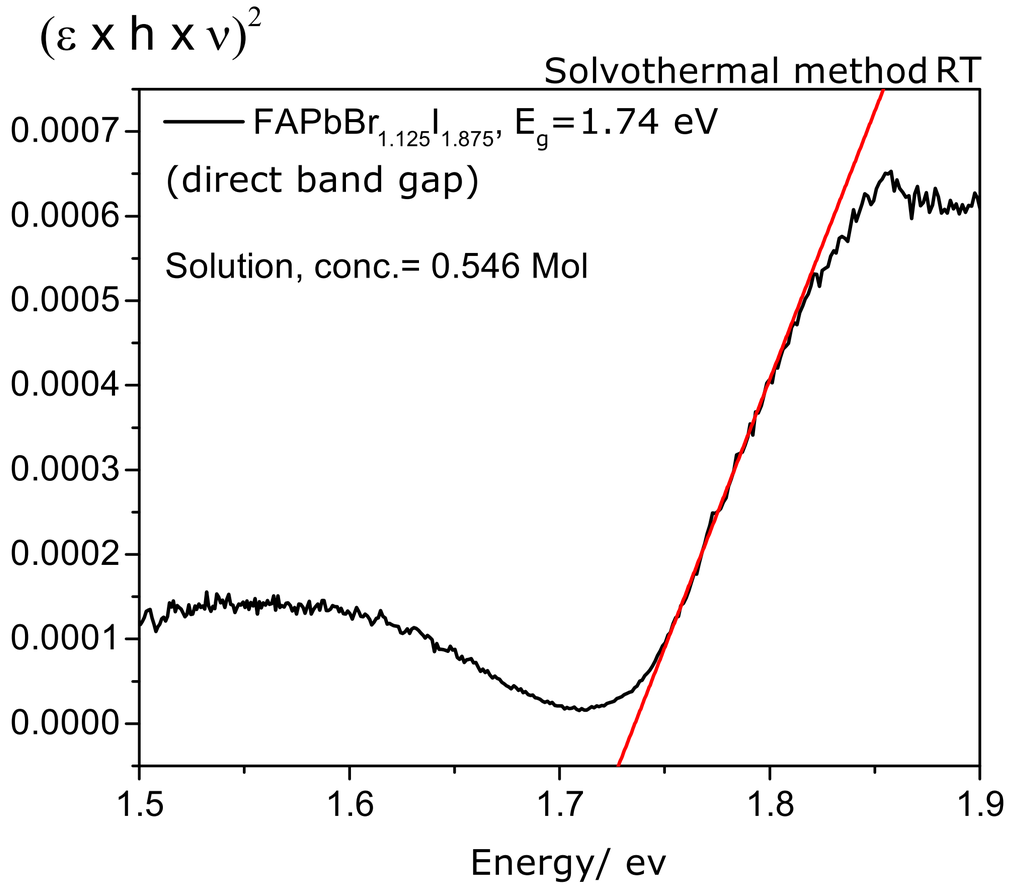
For that reason on the "x" axes $E = \frac{hc}{\lambda e}$ is placed in "ev", where "h" is Planck's constant, "c" is the speed of light, λ is the wavelength, and "e" is the exponent.

While on the "y" axes $(\varepsilon h\nu)^{\frac{1}{2}}$, where ε is the absorption coefficient, h is Planck's constant, ν is the wave frequency.

Band gap energy is found from intersection with "x" axes, taking into account the Tauc's relationship:

$(\varepsilon h\nu)^{\frac{1}{n}} = h\nu - E_g$, n=1/2 for direct bang gaps (for our case DFT calculations showed direct gap).

Tauc plot for $FAPb(Br_{0.375}I_{0.625})_3$ 12.08.2024



XRD results' from experiment: $FAPb(Br_{0.375}I_{0.625})_3$ sample and precursors 12.08.2024