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DFT Study of the Effect of A-Site and Halide Substitution on the Structural and Elastic Behavior of $APbX_3$ Perovskites

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ABSTRACT

In this study, density functional theory within the generalized gradient approximation – Perdew–Burke–Ernzerhof (GGA-PBE) was employed to examine the mechanical and structural characteristics of cubic $APbX_3$ (A = Li, Na, K, Rb, Cs; X = F, I) perovskites. Comparing the larger ionic size of iodides to fluorides, the optimized lattice parameters increase with the A-site ionic radius. The Born-Huang stability criteria are satisfied by all computed elastic constants, indicating mechanical stability in the cubic phase. Cubic $APbI_3$ perovskite compounds tend to have lower bulk moduli and are easily compressible, especially when the heavier A-site cations are present, while $APbF_3$ compounds show increased stiffness as bulk and Young's moduli increase from Li to Cs. Poisson ratios suggest predominantly ionic bonding across all compositions. Overall, fluoride perovskites are mechanically more robust than their iodide counterparts, highlighting the strong influence of both A-site and halide substitution on structure–mechanical property relationships.

Keywords:
GGA-PBE,
Lead halide perovskites,
Elastic constants,
Mechanical stability,
Structural properties.

INTRODUCTION

Lead halide perovskites ($APbX_3$) materials are attractive for optoelectronic (Kovalenko, Protesescu, & Bodnarchuk, 2017) and photovoltaic (Jishi, Ta, & Sharif, 2014) applications due to their promising light-absorption mechanism, tunable bandgaps, and relatively cost effective. All-inorganic cesium-based perovskites ($CsPbX_3$) are most studied in this class of material (Protesescu et al., 2015; Tan et al., 2023; Yang et al., 2019). This is because of their remarkable photovoltaic performance, with power-conversion efficiencies exceeding 22% (Laboratory, 2023). Cesium lead halides have good thermal and operational stability compared to hybrid organic–inorganic perovskites. This makes them better for long-term use in devices (Boote et al., 2019). Lead halide perovskites exhibit polymorphism with temperature-dependent phase transitions. Inorganic Cs-based perovskites and hybrid organic–inorganic systems, such as methylammonium and formamidinium lead halides, undergo structural transformations that modulate their bandgap, optical response, and structural stability (Alaei, Circelli, Yuan, Yang, & Lee, 2021; Huang, Bodnarchuk, Kershaw, Kovalenko, & Rogach, 2017).

Recent reviews have highlighted the chemical and structural origins of phase instability in $CsPbI_3$ and discussed various stabilization strategies, including A-site alloying, strain engineering, surface passivation, and additive incorporation, aimed at preserving optically active perovskite phases under operating conditions (Jin et al., 2024). Most previous studies concentrate primarily on electronic and optical properties, leaving the elastic response and zero-temperature mechanical stability trends across different A-site and halide chemistry insufficiently explored. Since elastic constants govern resistance to deformation, phase stability, strain tolerance, and defect formation, a clear understanding of their compositional dependence is crucial for rational materials design. Elastic constants and derived mechanical moduli such as bulk, shear, and Young's moduli, Poisson's ratio, and elastic anisotropy are not merely auxiliary material parameters, but are directly linked to structural phase stability, strain tolerance, defect formation, and device reliability. For cubic crystals, satisfaction of the Born mechanical stability criteria, ($C_{11} - C_{12} > 0$, $C_{11} + 2C_{12} > 0$, $C_{44} > 0$) (Born, Huang, & Lax, 1955), constitutes a necessary condition for mechanical stability. Violations of these criteria indicate elastic softening and an intrinsic tendency toward symmetry lowering, such as cubic-to-tetragonal or orthorhombic distortions, or other structural transformations. Experimentally, cesium lead halide perovskites ($CsPbX_3$, X = Cl, Br, I) are known to undergo temperature-driven structural phase transitions, evolving from low-symmetry orthorhombic or tetragonal phases to a high-symmetry cubic (α) perovskite phase at elevated temperatures (Hoffman et al., 2023). Temperature-dependent diffraction and spectroscopic measurements confirm the emergence of the cubic phase, while first-principles and molecular-dynamics simulations successfully reproduce the orthorhombic→tetragonal→cubic transition sequence and identify the cubic structure as the stable high-temperature polymorph (Yi et al., 2020). However, a recent study has shown that at ambient or low temperatures, optically active cubic and tetragonal iodide phases most notably $CsPbI_3$ are often only metastable and readily transform into non-perovskite yellow phases in the absence of external stabilization (Jin et al., 2024). Despite this, understanding the intrinsic mechanical stability of the cubic phase remains essential. While finite-temperature entropic effects, strain, pressure, or compositional tuning may stabilize the cubic structure experimentally, mechanical stability at zero temperature represents a fundamental prerequisite for its persistence, whether as a stable or metastable phase. In this context, first-principles study of elastic constants and mechanical stability criteria provides critical insight into cubic lead halide perovskites and offers a baseline for interpreting finite-temperature behavior and chemical stability. Therefore, the aim of this study is to investigate the effect of A-site cation size and halide substitution on the structural parameters and elastic properties of cubic $APbX_3$ perovskites using density functional theory within the GGA-PBE approximation. The objectives are to: (i) determine optimized lattice parameters and analyze compositional trends; (ii) compute elastic constants and verify Born mechanical stability criteria; (iii) evaluate derived mechanical moduli (bulk, Young's modulus, and Poisson ratio); and (iv) compare the relative mechanical robustness of fluoride and iodide systems. All calculations were performed at zero temperature and zero pressure. Spin–orbit coupling effects were neglected, as the primary focus of this study is on ground-state mechanical stability, which is generally less sensitive to SOC compared to electronic structure properties. The composition–structure–mechanical property relationships that can guide the design of mechanically stable lead halide perovskites is essential for A-site and halide chemistry control lattice strain, stiffness, and compressibility, this was with a view to provides fundamental insight necessary for stabilization strategies and long-term device reliability in optoelectronic and related applications.

MATERIALS AND METHODS

Computational Details

All calculations were performed using the plane-wave self-consistent field (PWscf) method within the DFT framework to investigate the structural and mechanical stability of cubic $APbX_3$ (A = Li, K, Cs, and Rb; X = F and I) perovskites. All simulations were performed using the plane-wave pseudopotential method as implemented in the Quantum ESPRESSO package (Giannozzi et al., 2009). The interaction between the valence electrons and ionic cores was described using the generalized gradient approximation (GGA), parameterized by Perdew–Burke–Ernzerhof (PBE) (Perdew & Zunger, 1981) of ultrasoft pseudopotentials, obtained from the official Quantum ESPRESSO pseudopotential repository ("Quantum ESPRESSO Project,"). The valence electronic configurations treated in the calculations are as follows: Li: [He] $2s^1$, K: [Ar] $4s^1$, Rb: [Kr] $5s^1$, Cs: [Xe] $6s^1$, Pb: [Pt] $6s^2 6p^2$, F: [He] $2s^2 2p^5$, I: [Pd] $5s^2 5p^5$. The Kohn–Sham wave functions were expanded in a plane-wave basis set, with kinetic energy cutoffs of 75 Ry chosen to ensure convergence of the total energy and stress within 10^{-6}Ry. The Brillouin zone was sampled using a Monkhorst–Pack k-point mesh of $7\times7\times7$, with a convergence at 0.1mRy energy threshold, optimized for the cubic unit cell to achieve accurate stress tensors and elastic constants. All $APbX_3$ (A = Li, K, Cs, and Rb; X = F and I) compounds were modeled in the ideal cubic perovskite structure with space group Pm3-m (No. 221). In this structure, the atomic positions are defined by the following Wyckoff coordinates: A-site cation (Li, K, Rb, Cs): (0, 0, 0), Pb atom: (½, ½, ½), X-site anions (F or I): (½, ½, 0), (½, 0, ½), and (0, ½, ½). These fractional atomic coordinates were used as the initial structural model for all calculations. During structural optimization, both the lattice parameters and atomic positions were fully relaxed while preserving the cubic symmetry. The optimized geometries were subsequently employed for the calculation of elastic constants and other mechanical properties. The elastic constants were determined using the stress–strain method, whereby small finite strains were applied to the relaxed structures and the corresponding stress responses were calculated self-consistently. Given primitive lattice vector which represent the unstrained, $\vec{a}$ lattice geometry for cubic structure

$$\vec{a} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \qquad (1)$$

The strained lattice vectors were transformed according to the applied strain tensor, and the total energy was computed for each deformation. The primitive vector $\vec{a}$ is transformed to $\vec{a}'$ under the mechanical strain as:

$$\vec{a}' = \vec{a}\,(I + \epsilon) \qquad (2)$$

I and ϵ are the Identity matrix and strain tensor, respectively. The strain tensor is related to the strain vector ϵ vector as (Wang & Ye, 2003)

$$\epsilon = \begin{pmatrix} \epsilon_1 & \epsilon_6/2 & \epsilon_5/2 \\ \epsilon_6/2 & \epsilon_2 & \epsilon_4/2 \\ \epsilon_5/2 & \epsilon_4/2 & \epsilon_3 \end{pmatrix} = \begin{pmatrix} \delta_1 & \delta_6 & \delta_5 \\ \delta_6 & \delta_2 & \delta_4 \\ \delta_5 & \delta_4 & \delta_3 \end{pmatrix} \qquad (3)$$

For convenience, we may express $\epsilon = \epsilon_n$ where n = 1, 2, 3, 4, 5 and 6 and $\epsilon = \{\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4, \epsilon_5, \epsilon_6\}$ are the the strain applied at different directions in the Voigt index notation. Following the ansatz, i.e., the relationship between the energy E of a solid crystal, applied strain, the corresponding volume V and the elastic constants C can be stated as:

$$\Delta E = \frac{V}{2}\sum_{j=1}^{6}\sum_{k=1}^{6} C_{jk}\epsilon_i \qquad (4)$$

Equation 4 can be expanded in Taylor series to any other on order to determine the appropriate energy-strain equation which can be fitted to obtain the corresponding elastic constants, as we shall below. Thus, we imposed specific strain vector in order to obtain the elastic constants. For example, the strain vector $\epsilon = \{\delta, 0, 0, 0, 0, 0\}$ gives the following expression for the deformation matrix

$$\vec{\boldsymbol{a}}' = \vec{a}\begin{pmatrix} 1+\delta & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad (5)$$

This is equivalent to applying elastic strain of magnitude δ along the [100] or x-direction. The corresponding energy-strain equation based on equation 4 is:

$$E(\delta) = E(0) + V_0(C_{11})\delta^2$$

To obtain the lattice constants, $C_{11}+C_{12}$, elastic strain vector $\epsilon = \{\delta, \delta, 0, 0, 0, 0\}$ is applied. The corresponding deformation matrix is:

$$\vec{\boldsymbol{a}}' = \vec{a}\begin{pmatrix} 1+\delta & 0 & 0 \\ 0 & 1+\delta & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad (6)$$

This is equivalent to applying elastic strain of magnitude, δ along the [100] and [010] direction. The energy-strain curve is fitted to the equation:

$$E(\delta) = E(0) + V_0(C_{11}+C_{12})\delta^2$$

C_{44}, is associated with shear deformation on planes normal to the principal axes of the deformation matrix, The corresponding deformation matrix for C_{44} is

$$\vec{\boldsymbol{a}}' = \vec{a}\begin{pmatrix} 1 & 0 & \delta \\ 0 & 1 & \delta \\ \delta & \delta & 1 \end{pmatrix} \qquad (7)$$

This is equivalent to applying elastic strain, δ on planes normal to the principal axis. The energy-strain curve is fitted to the equation:

$$E(\delta) = E(0) + 2V_0(C_{44})\delta^2 + V_0(\delta^4)$$

Strains δ ranging from -0.06 to 0.06, in steps of 0.01, were imposed on the lattice, and the corresponding total energies were obtained. Parabolic fit of energy versus strain were performed to obtain the elastic constants. The fitting were done using the simple Gnuplot (Racine, 2006). Having obtained the elastic constants, other key mechanical properties such as the shear modulus, Young's modulus, and Poisson's ratio, which collectively characterize the stiffness, ductility, fracture resistance, and directional dependence of elastic response. Shear modulus, G was obtained from

$$G = \frac{1}{2}(G_R + G_V) \qquad (8)$$

Where Voigt approximation, G_V and Reuss approximation G_C,

$$G_V = \frac{1}{5}(C_{11} - C_{12} + 3C_{44}), \quad \text{and} \quad G_R = \frac{5C_{44}(C_{11}-C_{12})}{4C_{44}+3(C_{11}-C_{12})},$$

Young modulus,

$$E = \frac{9B}{3B+G} \qquad (9)$$

The ratio of lateral strain to longitudinal strain under uniaxial deformation, poison ratio is obtained by,

$$\eta = \frac{2C_{44}}{(C_{11}-C_{12})} \qquad (10)$$

RESULTS AND DISCUSSION

The calculated lattice parameters of cubic $APbX_3$ (a = Li, Na, K, Rb, Cs; x = F, I) is shown in Table 1 using the GGA-PBE functional show clear systematic trends. For $APbF_3$, the lattice constant increases progressively from: $LiPbF_3$ (4.71 å), $NaPbF_3$ (4.75 å), $KPbF_3$ (4.76 å), $RbPbF_3$ (4.81 å), $CsPbF_3$ (4.81 å). This monotonic increase follows the ionic radius trend of the A-site cations ($Li^+ < Na^+ < K^+ < Rb^+ < Cs^+$). The expansion of the lattice with increasing A-site size is expected due to the enlargement of the cuboctahedral cavity within the perovskite framework. Similarly, for $APbI_3$, the lattice parameter increases from: $LiPbI_3$ (6.07 Å), $NaPbI_3$ (6.08 Å), $KPbI_3$ (6.31 Å), $RbPbI_3$ (6.54 Å), $CsPbI_3$ (6.57 Å). The lattice constants of iodides are significantly larger than those of fluorides, which is attributed to significantly larger ionic radius of I^- compared to F^-. This confirms that the X-site anion strongly influences structural expansion. Comparison with previously reported theoretical and experimental values shows good agreement, with only small deviations of GGA-PBE calculations, which are known to slightly overestimate lattice parameters due to the under binding nature of the functional.

Table 1: Calculated Lattice Parameters of Cubic Apbx3 (A = Li, K, Cs & Rb; X = F and I) Using the GGA-PBE

$APbF_3$	a (Å)	Ref	$APbI_3$	a (Å)	Ref
$LiPbF_3$	4.71)		$LiPbI_3$	6.07	
Others			Others	6.17	(Pakravesh & Izadyar, 2024)
$NaPbF_3$	4.75		$NaPbI_3$	6.08	
Others			Others	6.24	(Abdulla & Sami, 2023)
$KPbF_3$	4.76		$KPbI_3$	6.31	
Others			Others	6.33	(Abdulla & Sami, 2023)
$RbPbF_3$	4.81		$RbPbI_3$	6.54	
Others	4.87	(Hayatullah et al., 2013)	Others	6.31	(Jong, Yu, Kim, Kye, & Kim, 2018)
Exp.			Exp.		
$CsPbF_3$	4.81		$CsPbI_3$	6.57	
Others			Others	6.37	(Jong et al., 2018)

The calculated elastic constants (C_{11}, C_{12}, C_{44}) are shown in Table 2 for $APbF_3$ indicate: C_{11} increases steadily from Li to Cs. C_{12} and C_{44} also increase with increasing A-site ionic size. All compounds satisfy the Born–Huang mechanical stability criteria for cubic crystals: $C_{44} > 0$, $C_{11} - C_{12} > 0$, $C_{11} + 2C_{12} > 0$. This suggest that all $APbF_3$ compositions are mechanically stable in the cubic phase. The bulk modulus (B) increases from 41.20 GPa (Li) to 50.55 GPa (Cs), indicating increasing resistance to volume compression as the A-site cation becomes heavier. The Young's modulus (E) shows a similar increasing trend, implying enhanced stiffness from $LiPbF_3$ to $CsPbF_3$. The Poisson ratio (v) slightly decreases from 0.37 to 0.33. Since $v > 0.25$ for all compositions, the bonding character is predominantly ionic. The gradual decrease suggests a slight increase in directional bonding as the lattice expands.

Table 2: Calculated Elastic Constants (C_{11}, C_{12}, and C_{44}), *Born-Huang Conditions* (Y for Yes) and Mechanical Parameters (Bulk Modulus, Young Modulus, and Poisson Ratio) Of Cubic Apbf3 (A = Li, K, Cs & Rb) Using the GGA-PBE

Properties	$LiPbF_3$	$NaPbF_3$	$KPbF_3$	$RbPbF_3$	$CsPbF_3$
C_{11} (GPa)	94.74	96.23	98.91	102.06	106.8
C_{12} (GPa)	14.44	14.98	16.05	18.43	22.44
C_{44} (GPa)	3.26	4.15	6.37	7.85	10.50
Born-Huang Conditions					
$C_{44} > 0$	Y	Y	Y	Y	Y
$C_{11} - C_{12} > 0$	Y	Y	Y	Y	Y
$C_{11} + 2C_{12} > 0$	Y	Y	Y	Y	Y
Bulk Modulus, B	41.20	42.06	43.67	46.31	50.55
Young Modulus, E	31.77	34.39	40.41	44.32	50.86
Poisson ratio, u	0.37	0.36	0.34	0.34	0.33

The elastic behavior of $APbI_3$ presented in Table 3 shows more complex trends. C_{11} values is very high for $NaPbI_3$ (236.23 GPa) and moderate (~88–105 GPa) for others. C_{12} values are positive for Li and Na and slightly negative for K, Rb, and Cs. Although negative C_{12} values are unusual, the compounds still satisfy the Born–Huang criteria, indicating mechanical stability. Negative C_{12} may suggest unusual transverse response or anisotropic elastic behavior, which is sometimes observed in soft halide perovskites. Bulk modulus decreases significantly from Li/Na to K/Rb/Cs i.e. $LiPbI_3$: 46.09 GPa; $NaPbI_3$: 48.95 GPa, $CsPbI_3$: 27.44 GPa. This reduction indicates that heavier A-site iodides are more compressible and mechanically softer compared to their fluoride counterparts. With regards to Young's modulus, $NaPbI_3$ (67.95 GPa) show exceptionally high stiffness for while others are moderate with values, 39–43 GPa. Poisson ratio decreases from 0.37 (Li) to 0.23 (Cs), suggesting a gradual reduction in ionic character and possible increase in covalent contribution for heavier A-site iodides. Comparing Fluorides and Iodides perovskite compound, the lattice size of $APbI_3$ is greater than $APbF_3$ due to larger I^- ionic radius. Also, fluorides show more consistent and increasing stiffness across A-site substitution. Iodides become softer and more compressible as A-site size increases. In terms of the chemical bond, fluorides exhibit stronger ionic bonding (higher Poisson ratio), while the iodides are flexible and exhibit lower resistance to shear deformation. All compounds satisfy cubic mechanical stability conditions, confirming that the GGA-PBE optimized structures are mechanically viable.

Table 3: Calculated Elastic Constants (C_{11}, C_{12}, and C_{44}), *Born-Huang Conditions* (Y for Yes) and Mechanical Parameters (Bulk Modulus, Young Modulus, and Poisson Ratio) Of Cubic Apbi$_3$ (A = Li, K, Cs & Rb) Using the GGA-PBE

Properties	LiPbI$_3$	NaPbI$_3$	KPbI$_3$	RbPbI$_3$	CsPbI$_3$
C_{11} (GPa)	105.13	236.23	88.70	88.35	88.40
C_{12} (GPa)	16.57	19.16	-0.34	-1.58	-3.031
C_{44} (GPa)	3.77	4.56	6.06	6.82	8.0293
Born-Huang Conditions					
$C_{44} > 0$	Y	Y	Y	Y	Y
$C_{11} - C_{12} > 0$	Y	Y	Y	Y	Y
$C_{11} + 2C_{12} > 0$	Y	Y	Y	Y	Y
Bulk Modulus, B	46.094	48.95	29.33	28.39	27.44
Young Modulus, E	35.54	67.95	39.22	40.84	43.38
Poisson ratio, u	0.37	0.26	0.27	0.26	0.23

CONCLUSION

The structural and mechanical properties of cubic APbX$_3$ (A = Li, Na, K, Rb, Cs; X = F, I) were investigated using GGA-PBE calculations. The lattice parameters increase steadily with A-site ionic radius and are larger for iodides than fluorides. All compounds satisfy the Born–Huang stability criteria, confirming mechanical stability in the cubic phase. Fluoride perovskites exhibit higher bulk and Young's moduli, indicating greater stiffness, whereas iodide counterparts are comparatively softer and more compressible. The results highlight the strong influence of both A-site cation and halide substitution on the structure–mechanical property relationships of lead halide perovskites.

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