Electronic Supplementary Material (ESI) for Materials Advances.

Supporting Information

Exciton-Phonon Coupling in Alanine Base Hybrid Lead Bromide

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Table S1: Crystal data and details of the refinement $AlaPbBr_3.H_2O$.

Crystal data	$AlaPbBr_3.H_2O$
Empirical formula	$C_3H_{10}Br_3NO_3Pb$
Formula weight	555.04
Temperature [K]	298.0
Crystal system	monoclinic
Space group (number)	$C2$ (5)
a [Å]	21.8573(12)
b [Å]	6.0851(4)
c [Å]	8.7665(5)
α [°]	90
β [°]	93.367(2)
γ [°]	90
Volume [Å^3]	1163.97(12)
Z	4
ρ_{calc} [gcm^{-3}]	3.167
μ [mm^{-1}]	40.057
F(000)	984
Crystal size [mm^3]	0.124×0.097×0.057
Crystal colour	clear light yellow
Crystal shape	plate
Radiation	CuK_α (λ=1.54178 Å)
2Θ range [°]	10.11 to 136.26 (0.83 Å)
Index ranges	-26 ≤ h ≤ 26 -7 ≤ k ≤ 7 -10 ≤ l ≤ 10
Reflections collected	13066
Independent reflections	2075
$R_{indices}$	R_{int}=0.0473 R_{sigma} = 0.0342
Completeness to Θ = 67.679°	99.4 %
Data / Restraints / Parameters	2075/1/107
Goodness-of-fit on F2	1.101

Final R indexes	R1 = 0.0247
[I≥2σ(I)]	wR2 = 0.0633
Final R indexes	R1 = 0.0249
[all data]	wR2 = 0.0635
Largest peak/hole [eÅ−3]	1.01/-0.85
Flack X parameter	0.113(11)

Table S2: Bond parameters for $AlaPbBr_3.H_2O$ (in Å).

Atom 1-Atom 2...Atom 3	Atom 1-Atom 2	Atom 2...Atom 3
Pb1-Br2...N6 [i]	3.013(1)	3.327
Pb1-Br3...O3 [ii]	2.989(1)	3.365
Pb1-Br3...H3B [ii]	2.989(1)	2.575
Pb1-Br1...H6C [iv]	2.974(3)	3.024
N6-H6A...O3 [i]	0.890	2.714
N6-H6A...O1 [i]	0.890	1.978
N6-H6B...Br2 [i]	0.890	2.471
N6-H6C...Br2 [i]	0.890	2.613
C4-N6...Br2 [i]	1.49(1)	3.327
C3-O2...O3 [iii]	1.32(1)	2.600
C3-O2...H3A [iii]	1.32(1)	2.410
C3-O1...N6 [i]	1.19(1)	2.830
O2-H2...O3 [iii]	0.82	1.894
C5-H5B...O2 [iv]	0.96	2.531
C5-H5C...O1 [i]	0.96	2.668
O3-H3A...H2 [iii]	0.85	1.825
O3-H3B...Br3 [ii]	0.85	2.575
C3-C4	1.51(1)	
C4-H4	0.980	
C4-C5	1.51(2)	
C5-H5A	0.96	

Symmetry code: (i) 1/2-x,-1/2+y,1-z ; (ii) x,-1+y,z ; (iii) x,y,z; (iv) 1/2+x,1/2+y,z.

Table S3: Mode positions (centers, in cm^{-1}) and assignment of Raman spectrum of $AlaPbBr_3.H_2O$.

Wavenumber (cm^{-1})	Assignment	References
73, 86	L-Alanine lattice modes	[1]
79	δ_{as} (Br-Pb-Br)	[2–4]
101	υ_s (Br–Pb–Br)	
136	υ_s (Br-Pb)	
122	υ_{as} (Br-Pb).	
321	δ(CCNC)	[5–8]
394	δ(NCC)	
517	τ(NH_3)	[9]
541	r (CO_2)	
620	δ (CO_2)	
816	υ (CN)	[10,11]
1122	ρ (NH3)	
1207	ρ (CH3)	
1425, 1453	δas (CH3)	
1568	δas (NH3)	
1720	υ (CO2)	
2933	υ (NH3)	[11]
2950	υ (CH3)	
2993, 3019	υ (CH)	

Table S4: Bond lengths and angles for $[PbB_6]^{4-}$ octahedra of the organic-inorganic hybrid $AlaPbBr_3.H_2O$ crystal, as well as the calculated bond length quadratic elongation ($\langle\lambda\rangle$), and bond angle variance (σ^2).

Pb-Br Bond Length / Å	Br-Pb-Br Angle / degrees	
2.9740	98.37	85.12
3.1240	89.13	88.85
3.0131	87.26	93.42
2.9886	85.20	92.82
3.0352	93.59	88.25
3.0758	89.86	88.90
$\langle\lambda\rangle$=0.9602	σ^2=15.63	

Appendix 1

Split Pseudo-Voigt function

The fitting of PL curves and extracting their respective parameters were performed using the fityk software.[1].

Pseudo-Voigt function: Is a name given to the sum of Gaussian and Lorentzian functions:

$$y = a0\left[(1-a3)exp\left(-ln(2)\left(\frac{x-a1}{a2}\right)^2\right) + \frac{a3}{1+\left(\frac{x-a1}{a2}\right)^2}\right]$$

Here, long parameter names (like "height", "center" and "hwhm") were replaced with ai. In this case, a2 is half width at half maximum (HWHM=FWHM/2, where FWHM stands for full width…), which is proportional to the standard deviation: $a2 = \sqrt{2ln2}\sigma$.

Split Pseudo-Voigt function are used when the peak is noticeably asymmetric:

$$y(x;a0,a1,a2,a3,a4,a5) = \begin{cases} PseudoVoigt\ (x;a0,a1,a2,a4), & x \le 1 \\ PseudoVoigt\ (x;a0,a1,a3,a5), & x > 1 \end{cases}$$

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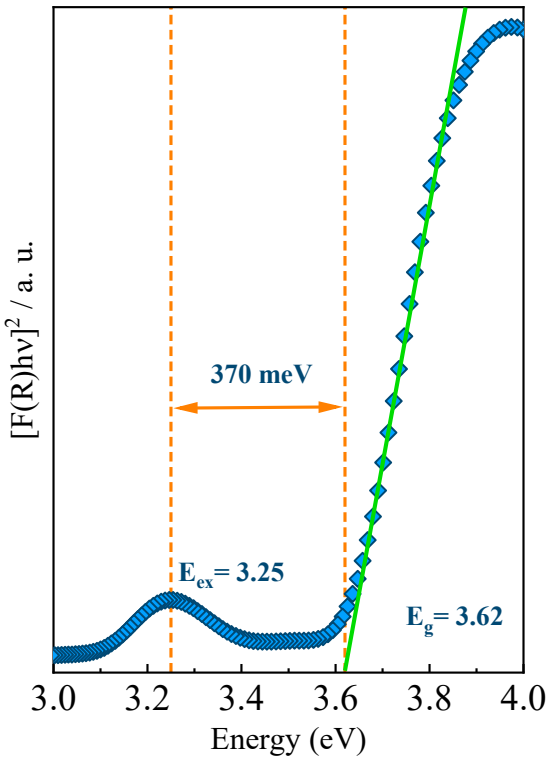

Figure S1: Exciton binding energy determination. The exciton binding energy was estimated taking the difference between the energy of the excitonic transition and the onset of the high-energy absorption band.

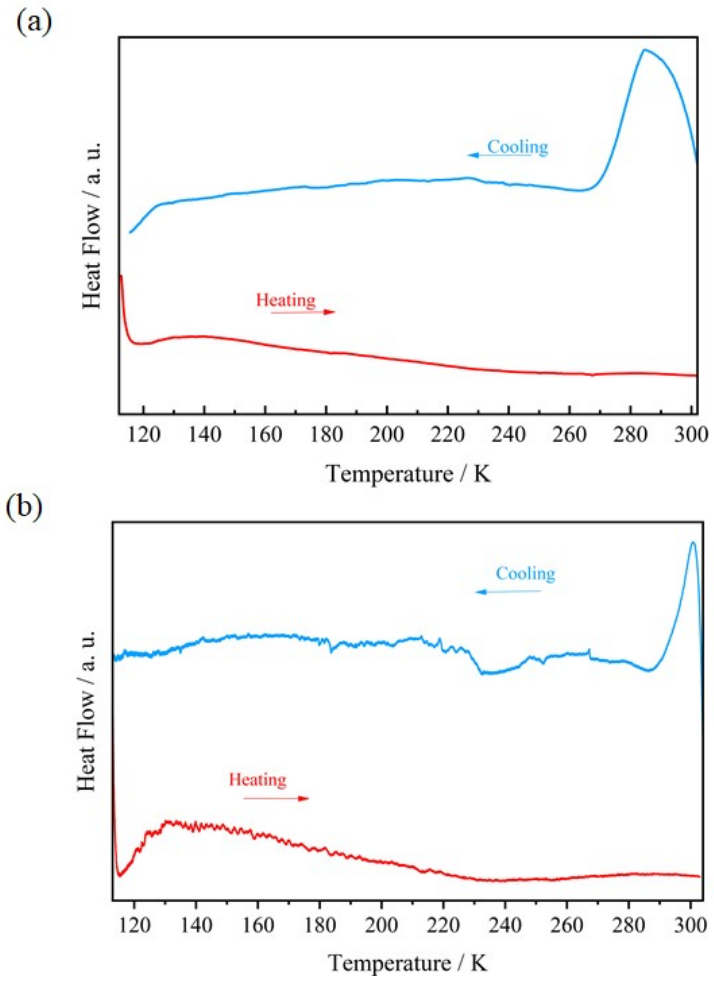

Figure S2: DSC thermogram of $AlaPbBr_3.H_2O$ single crystals from 120 K up to 300 K in a) 10K/ min rate and b) 5K/min rate.

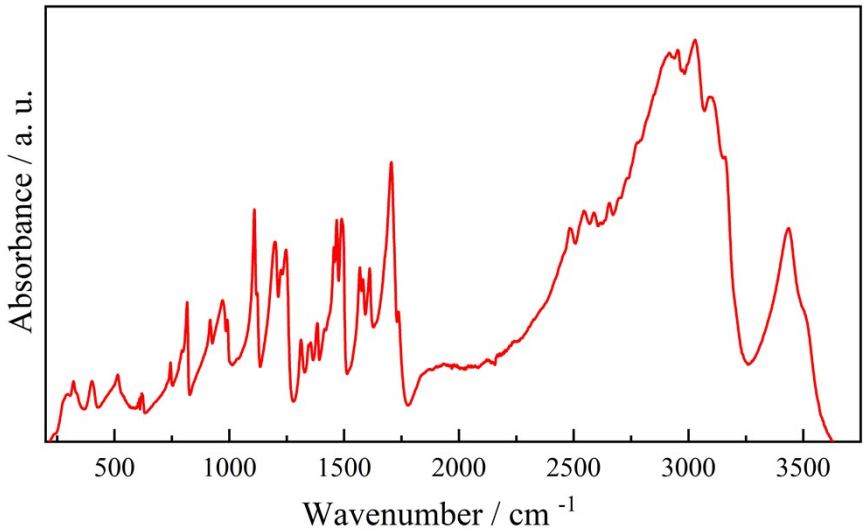

Figure S3: ATR-FTIR spectrum of $AlaPbBr_3.H_2O$ at 300 K.

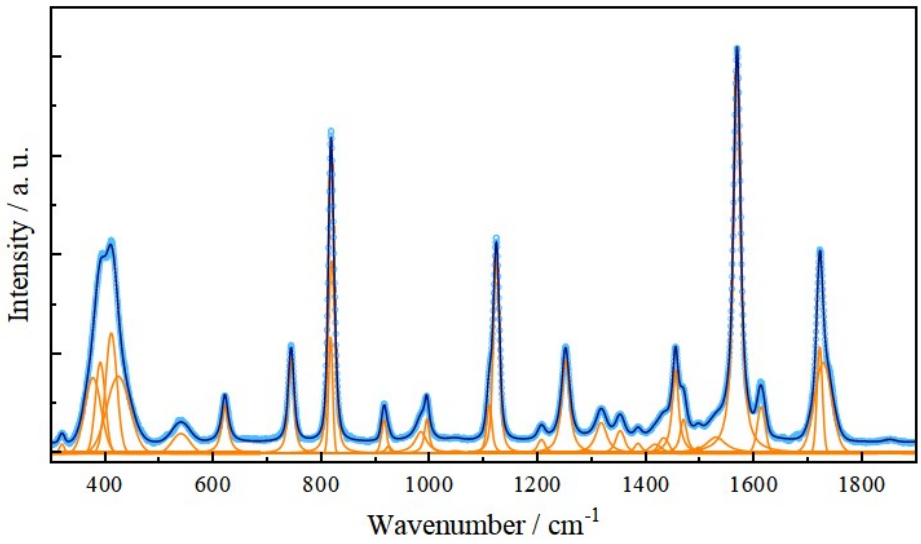

Figure S4: Intermediate-wavenumber region of the unpolarized Raman spectrum for $AlaPbBr_3.H_2O$ crystals, measured with a 633 nm laser line at room temperature.

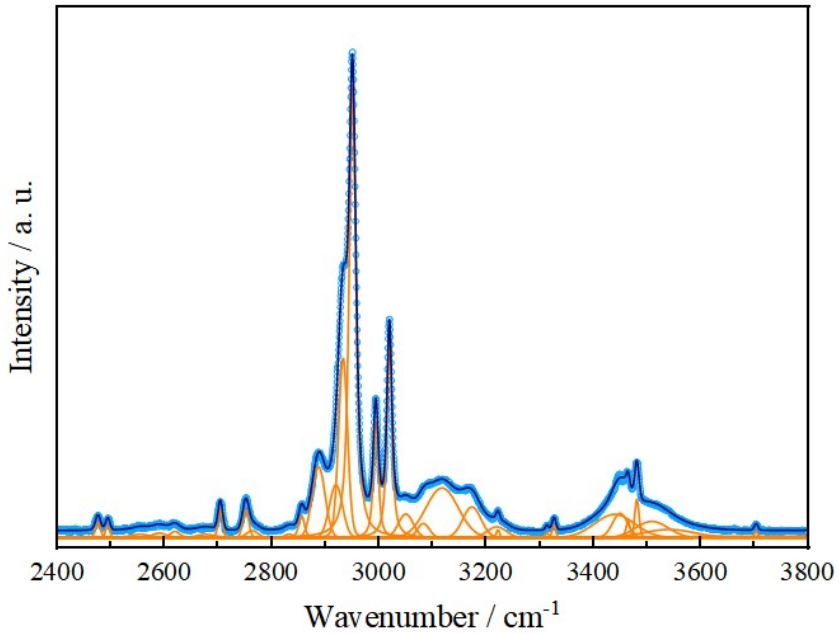

Figure S5: High-wavenumber region of the unpolarized Raman spectrum for $AlaPbBr_3.H_2O$ crystals, measured with a 633 nm laser line at room temperature.