

Digital flow platform for the synthesis of high-quality multi-material perovskites

Diego Iglesias,^a Christopher Tinajero,^a Simone Marchetti,^a Jaume Luis-Gómez,^b Raúl Martínez-Cuenca,^b Jose F. Fuentes-Ballesteros,^b Clara A. Aranda,^c Alejandro Martínez Serra,^d María C. Asensio^{e,f} Rafael Abargues,^d Pablo B. Boix,^g Marcileia Zanatta,^{a,h} Victor Sans*^a

^a Institute of Advanced Materials (INAM), Universitat Jaume I, Avda Sos Baynat s/n, 12071, Castellón, Spain

^b Department of Mechanical Engineering and Construction, Universitat Jaume I, 12071, Castellon, Spain

^c Center for Nanoscience and Sustainable Technologies (CNATS), Department of Physical, Chemical and Natural Systems, Universidad Pablo de Olavide, 41013, Seville, Spain

^d Instituto de Ciencia de los Materiales de la Universidad de Valencia (ICMUV), Valencia, 46980 Spain

^e Materials Science Institute of Madrid (ICMM/CSIC), Cantoblanco, E-28049 Madrid, Spain

^f MATINÉE, the CSIC Associated Unit between the Materials Science Institute (ICMUV) and the ICMM, Cantoblanco, E-28049 Madrid, Spain

^g Instituto de Tecnología Química, Universitat Politècnica València-Consejo Superior de Investigaciones Científicas, Av. dels Tarongers, València, 46022, Spain

^h Departament de Química Física i Analítica, Universitat Jaume I, Av. Sos Baynat s/n, 12071 Castelló de la Plana, Spain

Additional information of the flow platform.

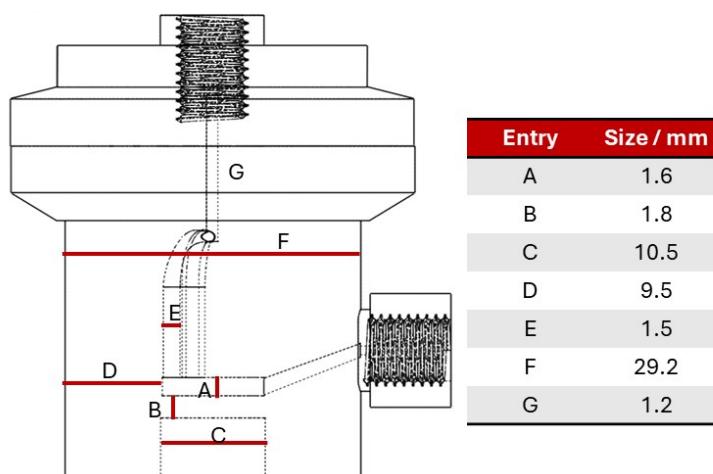


Figure S1. Detailed measurements of the 3D-printed reactor

Temperature control

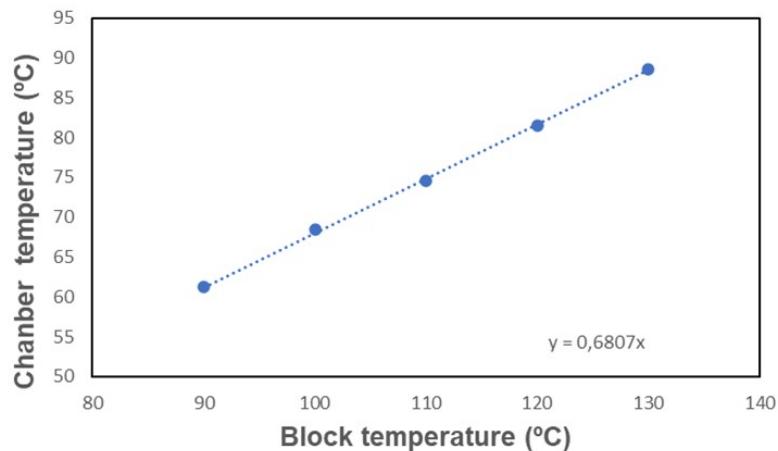


Figure S2. Temperature calibration.

$$y=0.68 \cdot x. R^2=0.999 \quad \text{Eq. S1}$$

Monitored growth of perovskite single crystals experiments

Table S1. Conditions used in growth monitoring experiments

Entry	Concentration (M)	T heater (°C)	Flow ($\mu\text{L/min}$)
1	1.2	85	25
2	1.2	85-95	25
3	1.2	90	25
4	1.2	90	12,5
5	1.2	90	50
6	1.2	95	25
7	1.2	100	25

Characterization of synthesized perovskite single crystals

Table S2. XRD data corresponding to MAPbBr_3 perovskite single crystals

Entry	hkl	2θ (°)	b (°)	θ (°)	θ (rad)	b (rad)	$\cos \theta$	$\sin \theta$
1	0 0 1	14,972	0,06729	7,486	0,131	0,00117	0,991	0,130
2	0 0 2	30,140	0,06732	15,070	0,263	0,00117	0,966	0,260
3	0 0 3	45,887	0,06330	22,944	0,400	0,00110	0,921	0,390

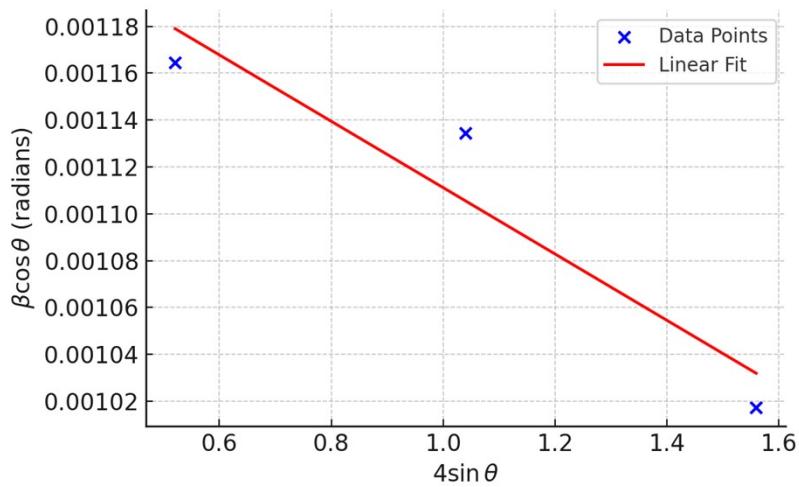


Figure S3. Williamson-Hall plot corresponding to the MAPbBr_3 perovskite. $y = -1.4 \cdot 10^{-4}x + 1.25 \cdot 10^{-3}$. $R^2 = 0.895$

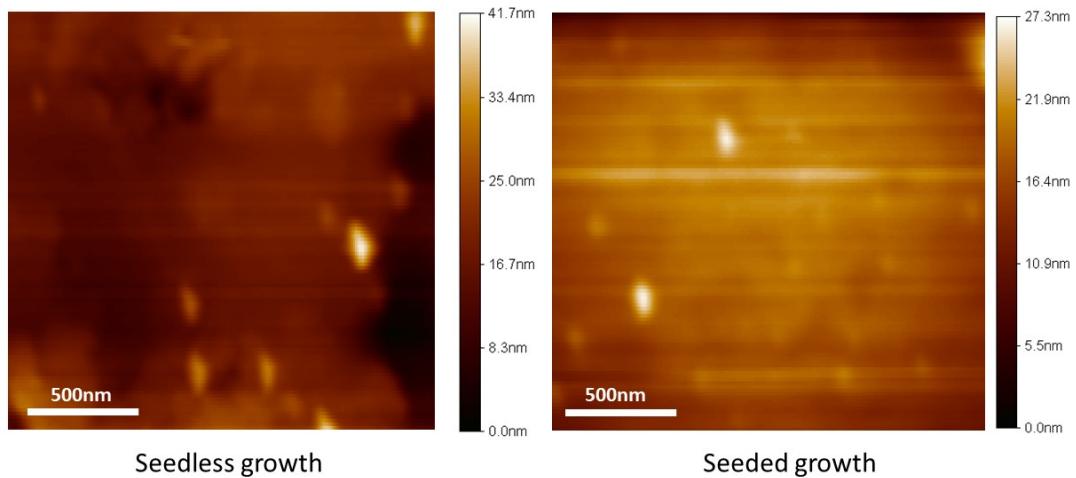


Figure S4. Atomic Force Microscopy images of grown crystals

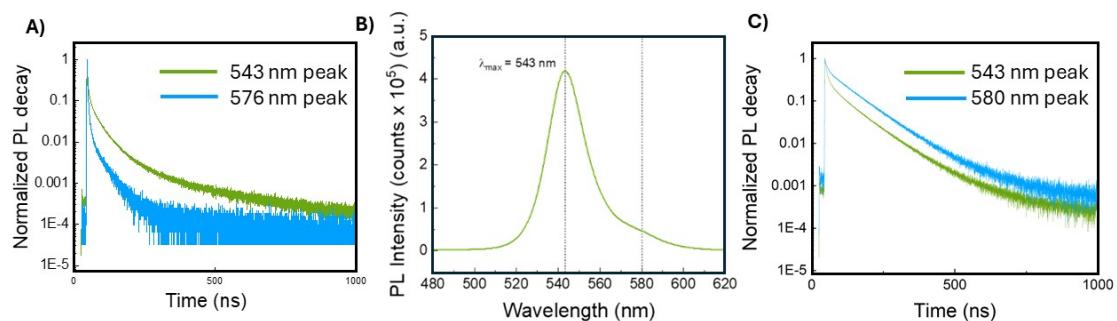


Figure S5. A) TRPL measurement of methylammonium lead bromide perovskite single crystal grown without seed. The lifetimes corresponding to both are shown in Table S3 B) PL spectra of a MAPbBr_3 perovskite single crystal grown using seeds. C) TRPL measurement of MAPbBr_3 perovskite single crystal grown without seed.

Table S3

Sample	τ_1 (ns)	τ_2 (ns)	τ_3 (ns)
543 nm peak (Unseeded)	9.04	39.8	181.7
576 nm peak (Unseeded)	5.9	36.7	152
543 peak (Seeded)	6.57	31.33	91.31
580 peak (Seeded)	7.77	60.02	101.94

Growth of mixed composition perovskite single crystal

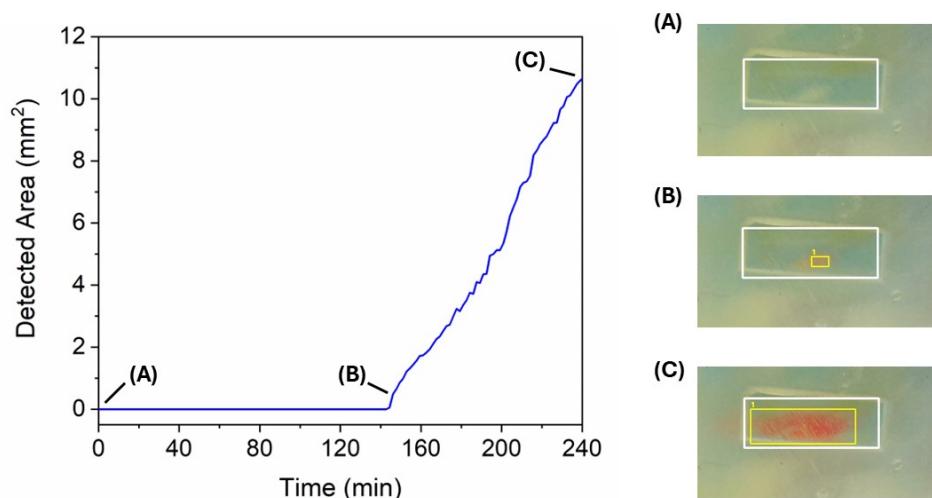


Figure S6. Growth kinetics of mixed composition single crystal

Characterization of synthesized mixed composition single crystal perovskites

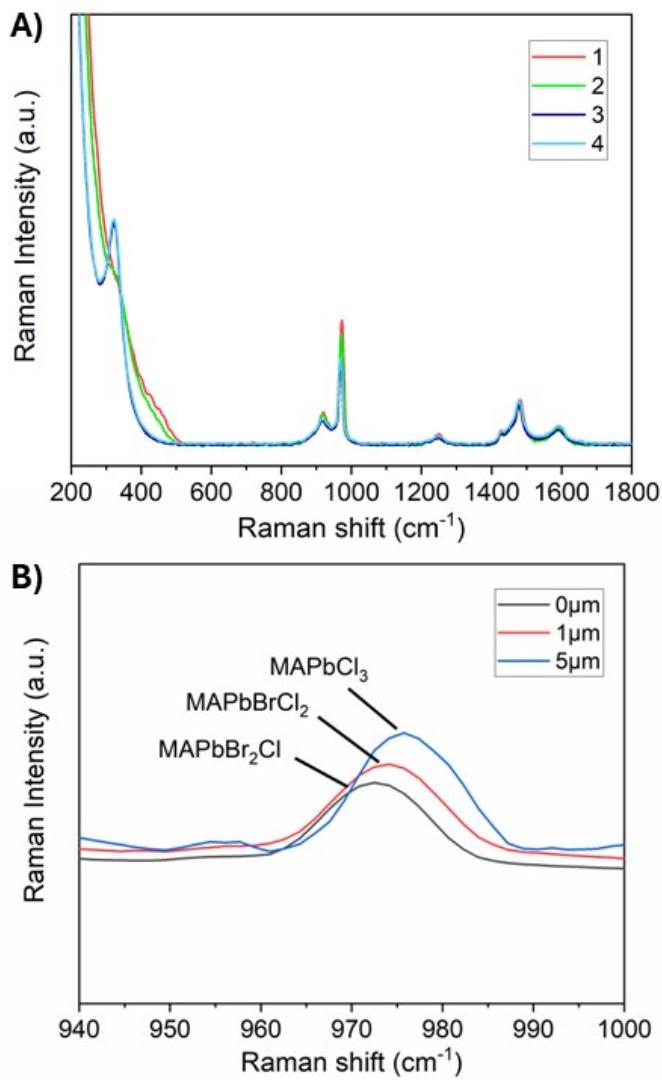


Figure S7. A) Raman spectra of different points of crystal surface. B) Raman shift measurements at the center of the crystal at surface, 1 μm under surface and 5 μm under surface.

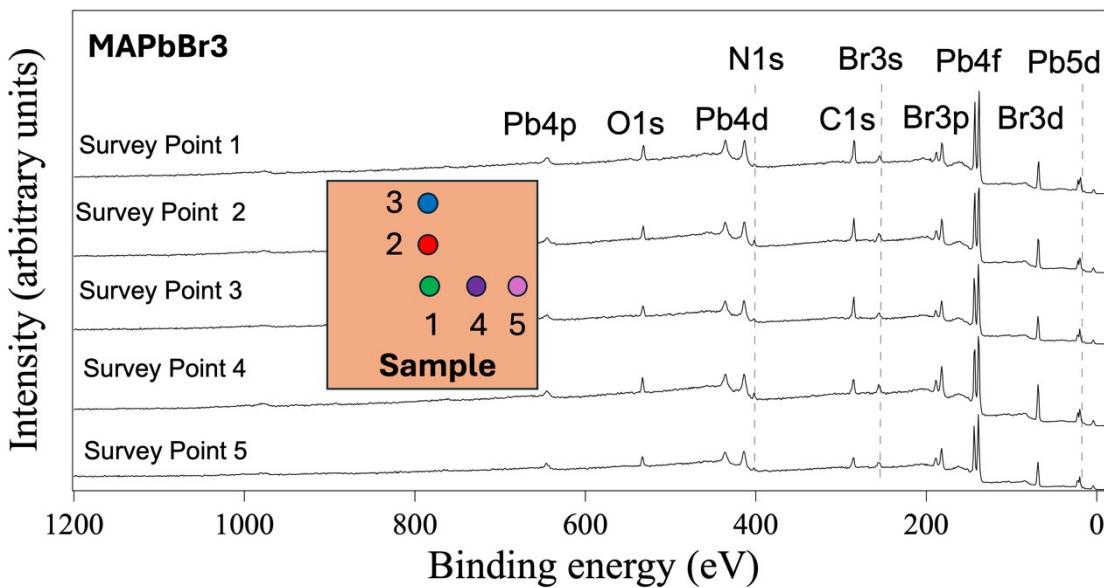


Figure S8. XPS survey spectra from five different positions on the sample, as indicated in the inset. The core levels of Pb, C, Br, N, and O confirm the spectroscopic homogeneity of the top perovskite film, MAPbBr_3 , with no detectable chlorine core level signals.

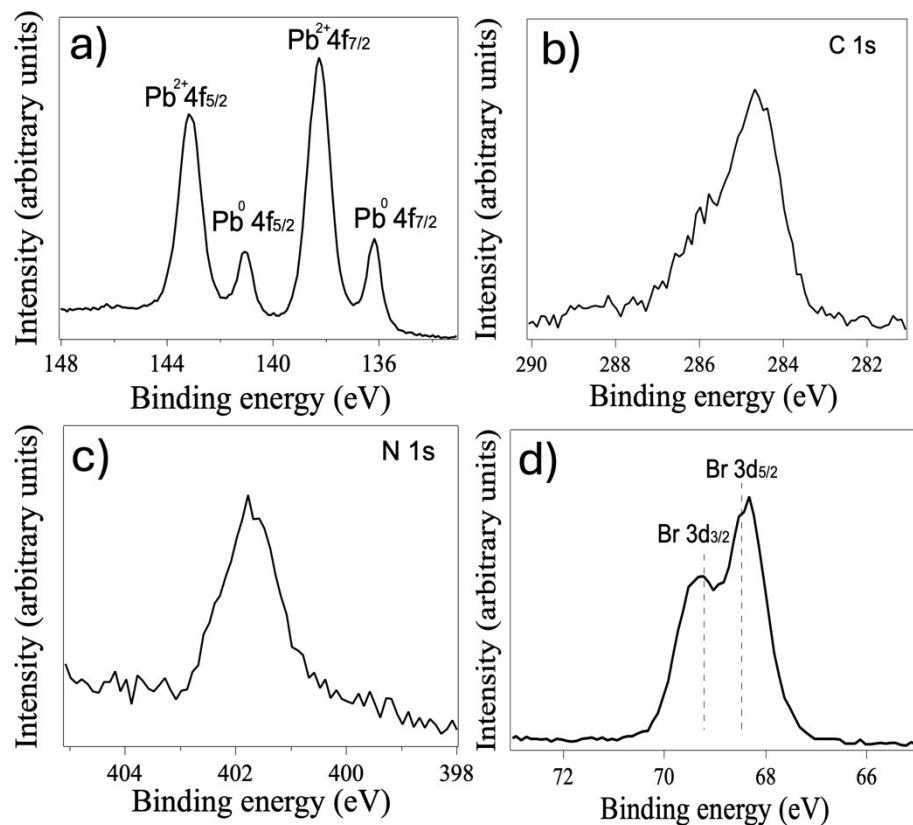


Figure S9. High-resolution XPS spectra of the a) Pb 4f, b) C 1s, c) N 1s, and d) Br 3d peaks measured at point 1 on the sample, as indicated in the inset of Figure 6.

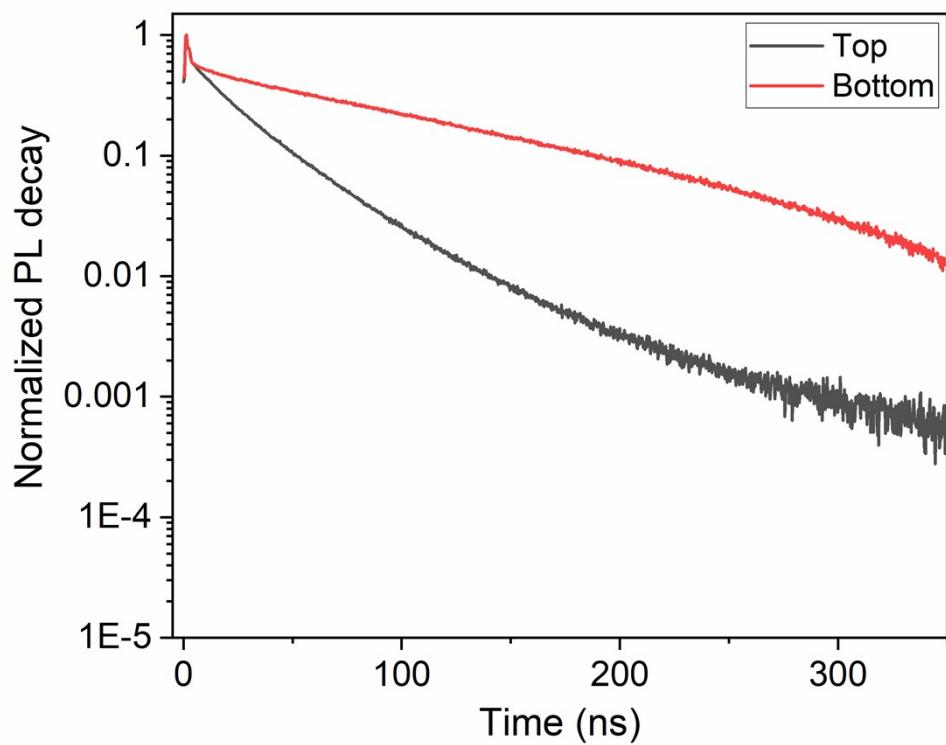


Figure S10. Normalized PL decay comparing the two faces. The lifetimes corresponding to both are shown in Table S4

Table S4. Photoluminescence decay times for mixed composition crystals

Sample	τ_1 (ns)	τ_2 (ns)	τ_3 (ns)	τ_{avg} (ns)
Top	1.2	12.3	125	46.6
Bottom	1.2	17.8	41.7	20.2

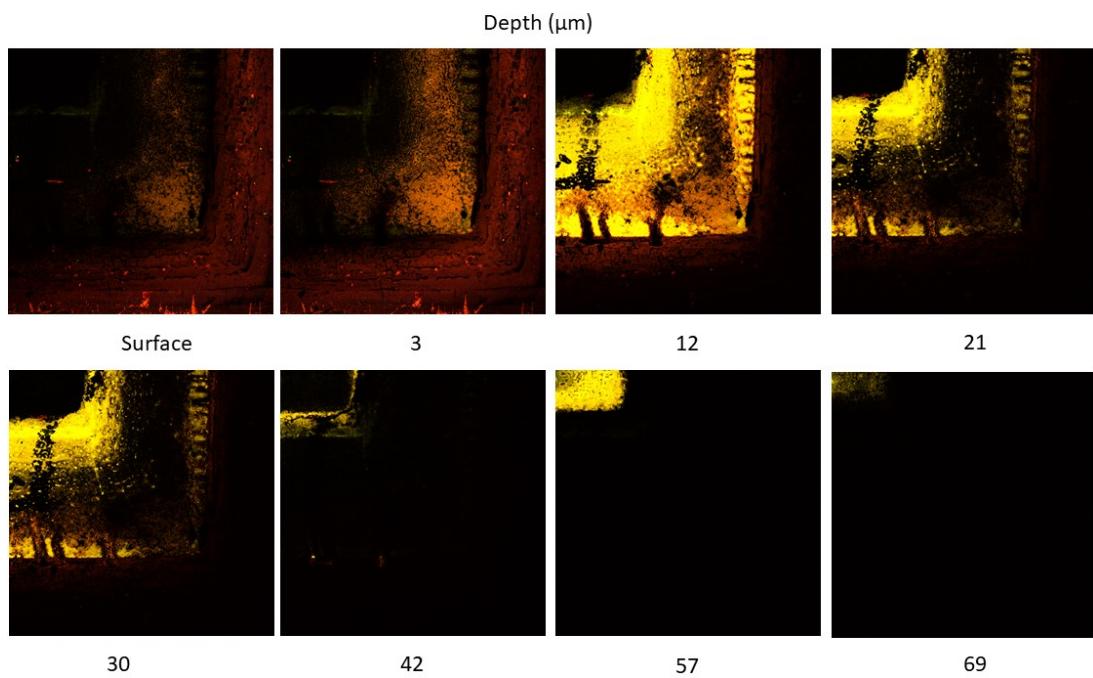


Figure S11. Photoluminescence microscopy image at different depths

Table S5. Channel wavelength range used in confocal photoluminescence images.

Channel	Wavelength range (nm)
1 (MAPbCl ₃ , white)	408-428
2	433-453
3	458-478
4 (Yellow)	482-501
5	507-517
6	527-537
7(MAPbBr ₃ , red)	547-557