Supplementary Material for
"Utilization of Complexity to Quantify the Regularity and Stochasticity of Nanocrystal Structure"

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Power spectral density (PSD) is a common measure used in structural analysis. It is calculated based on Fourier transformation. The Lorentz correction method can be used to accurately confirm the peak position of PSD. It calculates q^2I and plots the curve of q^2I with respect to q. As shown in Fig. S2b, the peaks of $CsPbBr_3$ at $-140°C$ and $CsPbBr_3$ at $-180°C$ were 0.501 and 0.140, respectively.
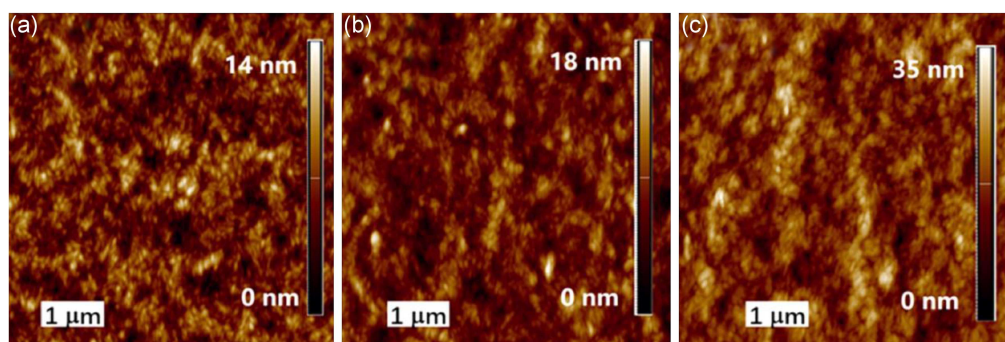

Fig. S1.   Atomic force microscopy (AFM) height images of PBDB-T/ITIC films with (a) 0% DIO, root-mean-square (RMS) roughness = 2.61 nm; (b) 0.5% DIO, RMS = 3.37 nm; (c) 1% DIO, RMS = 4.08 nm; reprinted from *Appl. Mater. Interfaces* **12** (2020) with permission. Copyright 2020 American Chemical Society.
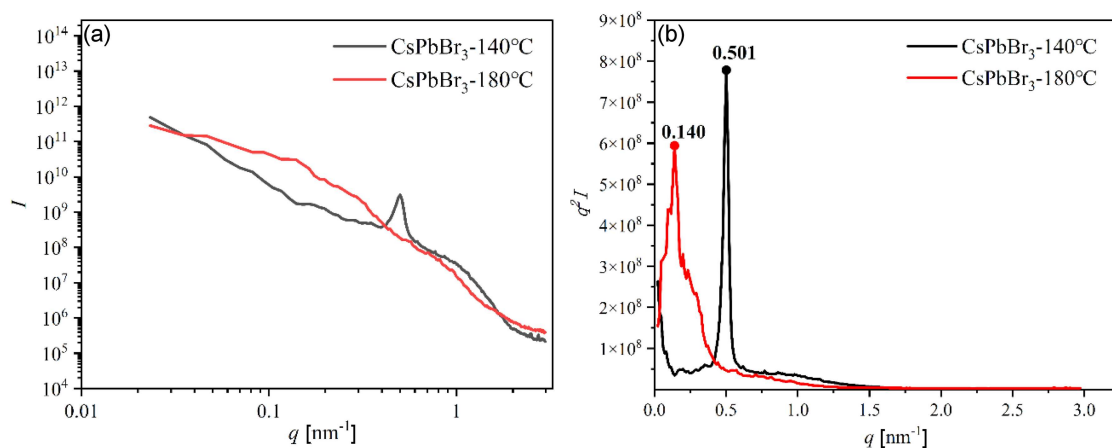

Fig. S2.   (a) Power spectral density (PSD) calculated by Fourier-transformation and (b) Lorentz correction of PSD for sample $CsPbBr_3$ at $-140°C$ and sample $CsPbBr_3$ at $-180°C$.

Fig. S3.   Sample CsPbBr$_3$ at -140°C. (a) Original image and images at the different coarse-graining scale: (b) coarse-graining scale = 2, (c) coarse-graining scale = 4, (d) coarse-graining scale = 8, (e) coarse-graining scale = 16, (f) coarse-graining scale = 32, (g) coarse-graining scale = 64, (h) coarse-graining scale = 128, and (i) coarse-graining scale = 256.
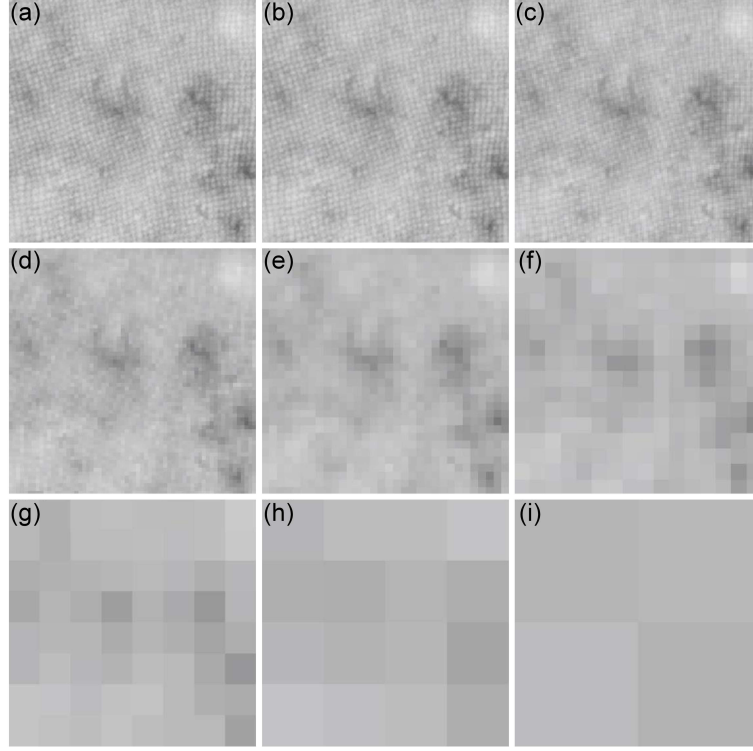

Fig. S4.   Sample CsPbBr$_3$ at -180°C. (a) Original image and images at the different coarse-graining scale: (b) coarse-graining scale = 2, (c) coarse-graining scale = 4, (d) coarse-graining scale = 8, (e) coarse-graining scale = 16, (f) coarse-graining scale = 32, (g) coarse-graining scale = 64, (h) coarse-graining scale = 128, and (i) coarse-graining scale = 256.
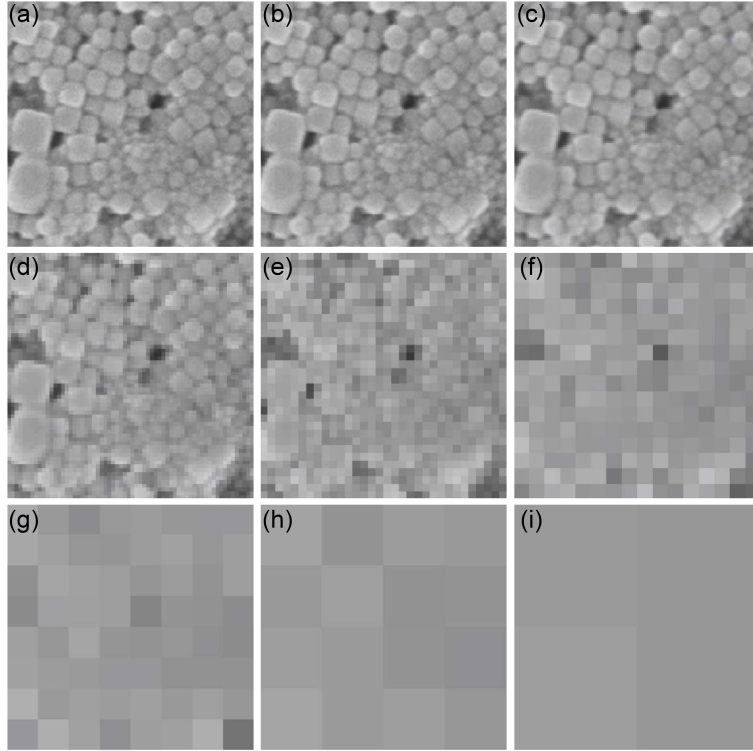
Entropic complexity and compression ratio of different samples as the coarse-graining scale changes.

| Coarse-graining scale [pixel]	CsPbBr$_3$			CsPbBr$_x$I$_{3-x}$			CsPbBr$_x$Cl$_{3-x}$		
	-140°C	-160°C	-180°C	-140°C	-160°C	-180°C	-140°C	-160°C	-180°C
	Fig. 1a	Fig. 1b	Fig. 1c	Fig. 1d	Fig. 1e	Fig. 1f	Fig. 1g	Fig. 1h	Fig. 1i
Entropic complexity									
2^1	6.2227	7.4551	6.6686	6.6741	6.3683	7.3237	6.5183	6.3854	7.0267
2^2	6.1532	7.4367	6.6386	6.6317	6.3274	7.2841	6.4572	6.3551	6.9945
2^3	5.9859	7.3819	6.5458	6.5342	6.2242	7.1529	6.3131	6.2739	6.9004
2^4	5.8238	7.2317	6.2873	6.3761	6.0078	6.7916	6.0955	6.0577	6.6436
2^5	5.5096	6.7633	5.6891	6.1054	5.6496	6.1202	5.7363	5.6737	6.1189
2^6	4.9784	5.5702	4.7703	5.3709	4.9681	4.9784	5.1480	4.7612	4.8980
2^7	3.4528	3.8750	3.4528	3.7500	3.8750	3.6250	3.6250	3.6250	3.5000
2^8	2.0000	2.0000	2.0000	2.0000	2.0000	1.5000	1.5000	2.0000	1.5000
Compression ratio									
2^1	0.2079	0.2083	0.1969	0.2096	0.2006	0.2378	0.2167	0.1965	0.2130
2^2	0.0507	0.0508	0.0507	0.0516	0.0501	0.0571	0.0527	0.0496	0.0530
2^3	0.0150	0.0159	0.0162	0.0156	0.0157	0.0176	0.0159	0.0157	0.0168
2^4	0.0058	0.0060	0.0061	0.0059	0.0059	0.0063	0.0059	0.0060	0.0062
2^5	0.0030	0.0031	0.0031	0.0031	0.0031	0.0031	0.0031	0.0031	0.0031
2^6	0.0020	0.0021	0.0021	0.0021	0.0021	0.0021	0.0020	0.0021	0.0021
2^7	0.0036	0.0039	0.0037	0.0035	0.0035	0.0037	0.0037	0.0038	0.0037
2^8	0.0018	0.0019	0.0017	0.0018	0.0018	0.0017	0.0018	0.0017	0.0018
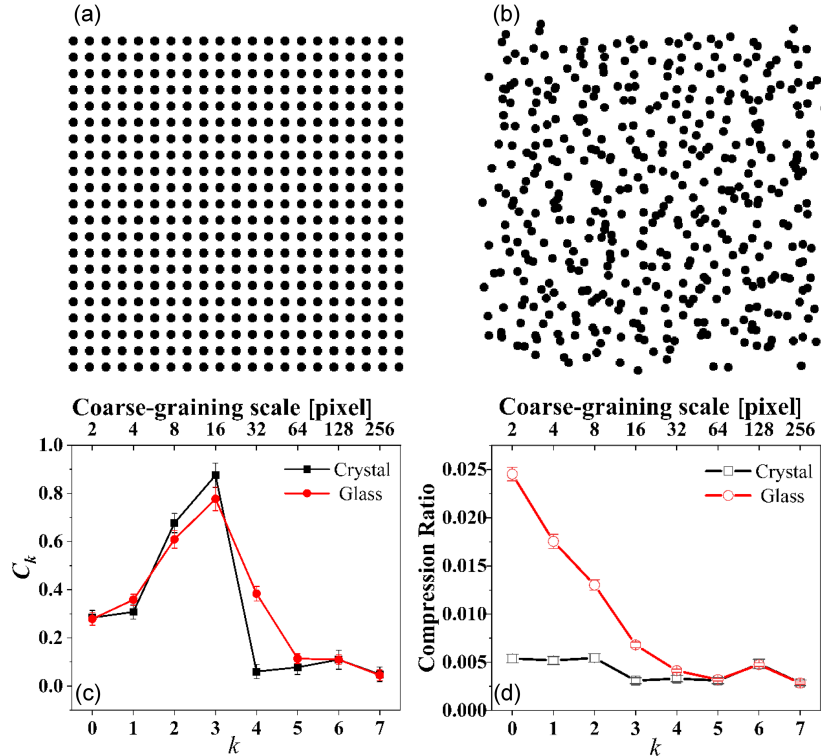
Fig. S5. Representation of (a) crystal structure and (b) glass structure; (c) partial complexity C_k of crystal and glass as a function of coarse-graining scale; (d) partial compression ratio of crystal and glass as a function of coarse-graining scale. The total values of structural complexity for the crystal structure and glass structure are 2.44 and 2.68, respectively. The values of compression ratio for the original crystal structure and glass structure are 0.005729 and 0.026852, respectively.