Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Information for

Oriented UiO-66 Thin Films through Solution Shearing

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Integrated GIXD patterns of UiO-66 films with various concentrations of benzoic acid modulator

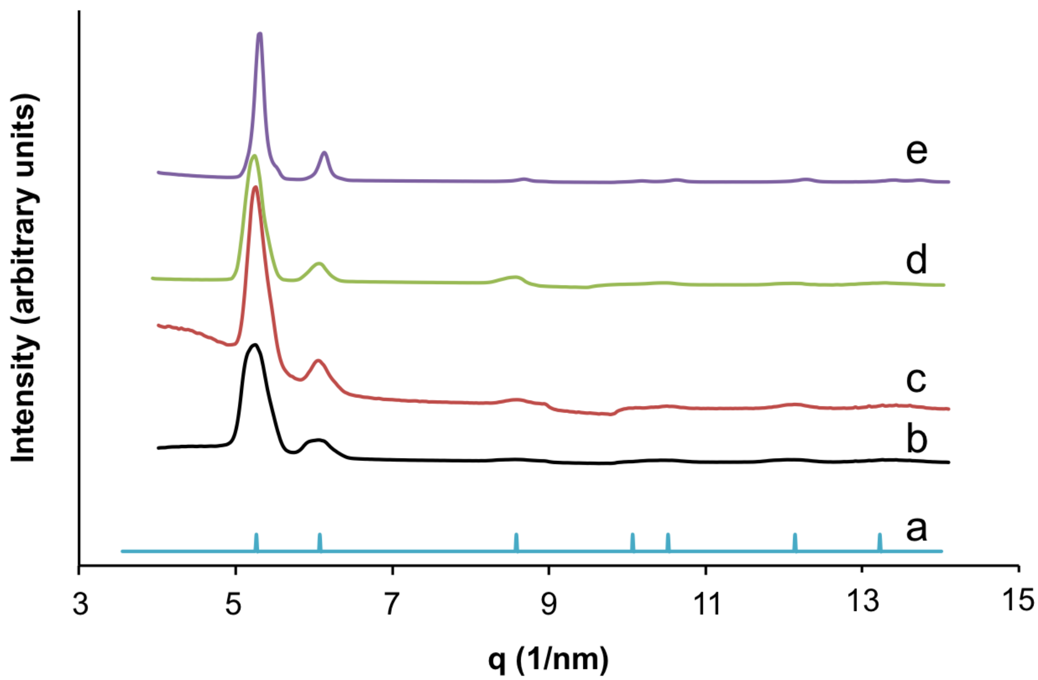

Fig. S1 a) Simulated PXRD pattern of UiO-66[1] and integrated GIXD patterns of UiO-66 crystals prepared from synthesis solutions with: b) 0, c) 40, d) 80 eq. benzoic acid as modulator and sheared on UV-ozone treated silicon wafers at 130 °C and 0.25 mm/s blade speed, and e) 80 eq. benzoic acid as modulator and dropcast on a UV-ozone treated silicon wafer at 130 °C. DMF was used as solvent in all cases.

'Cake' integration of the 2D GIXD pattern to quantify degree of UiO-66 film orientation

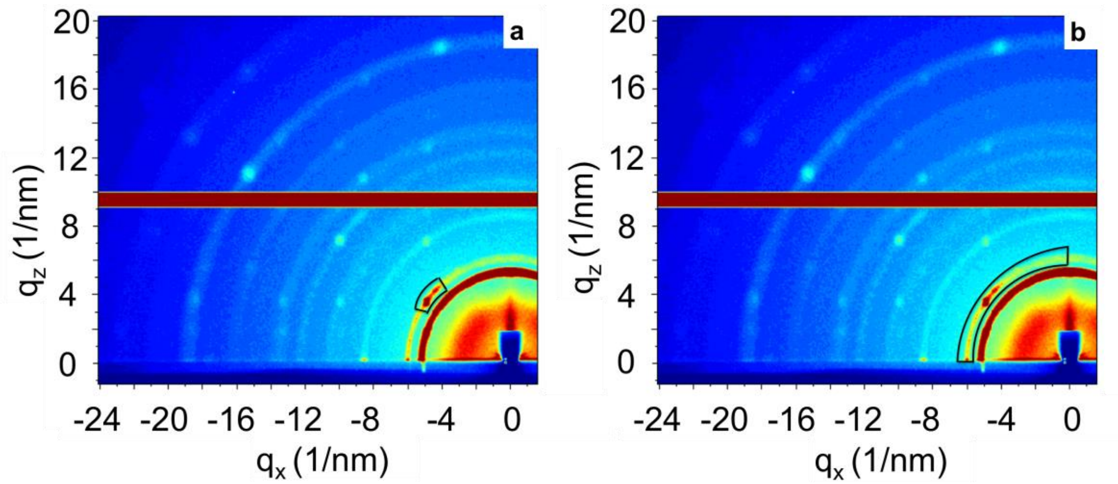

Fig. S2 a) A highly oriented region and b) the entire diffraction quarter ring, marked with black arcs depict the regions whose intensities are used to calculate orientation numbers. The same regions were used to characterize the non-oriented films.

Film thickness characterization

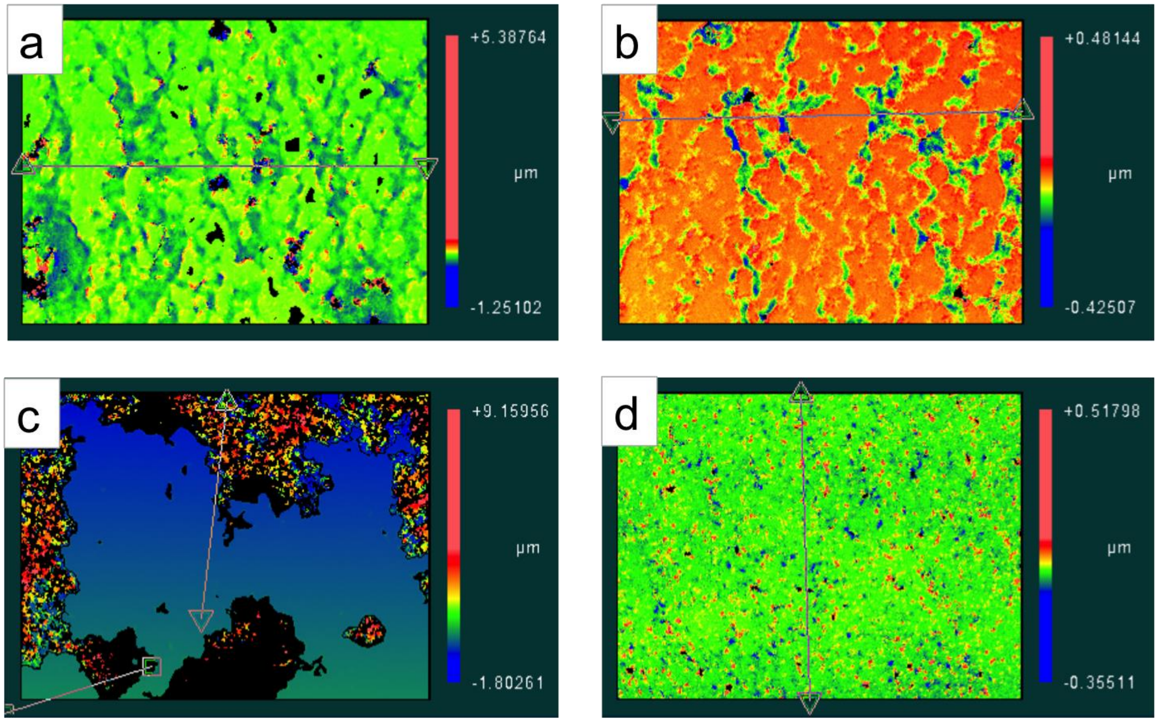

Fig. S3 Interferometry results of films made of UiO-66 particles modulated with 0 and 80 eq. benzoic acid and sheared at 0.1 and 0.25 mm/s at a temperature of 130 °C, on a UV-ozone treated silicon substrate with DMF as solvent. a) 0 eq, 0.1 mm/s, b) 0 eq, 0.25 mm/s, c) 80 eq., 0.1 mm/s, d) 80 eq., 0.25 mm/s.

Effect of substrate functionalization on UiO-66 film orientation

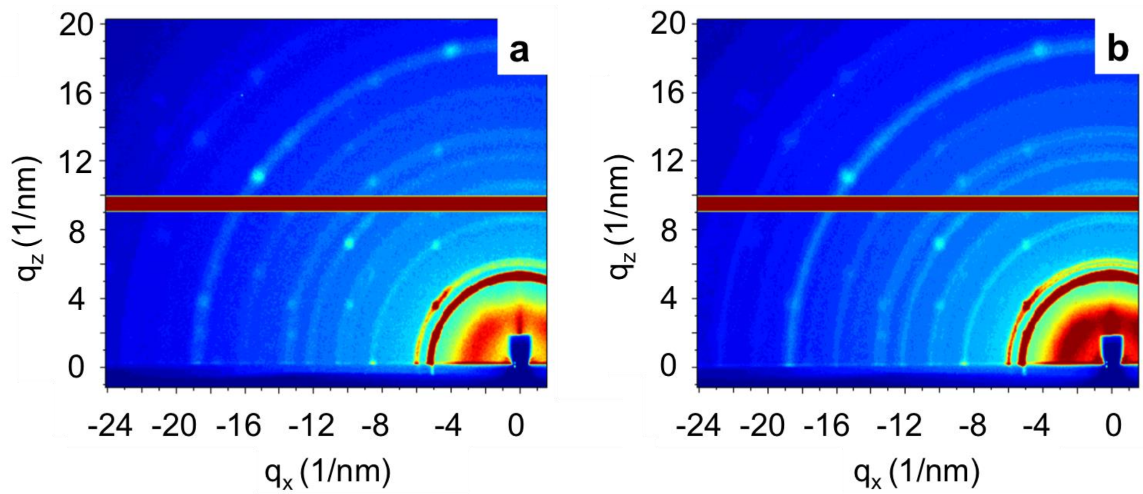

Fig. S4 2D GIXD patterns of 80 eq. benzoic acid modulated UiO-66 crystals sheared on: a) unmodified and b) PTS-treated silicon wafers at 130 °C and 0.25 mm/s blade speed, with DMF as solvent. Crystal orientation is observed with both substrates.

Orientation numbers of UiO-66 thin films

Table S1. Orientation numbers of UiO-66 thin films prepared at various crystallization and shearing conditions.

Sample	Synthesis time (hr)	Modulator type	Modulator concentration (eq.)	Substrate surface functionalization	Shearing solvent	Shearing temperature (°C)	Shearing blade speed (mm/s)	Orientation number
1	6	benzoic acid	80	UV-ozone	DMF	130	0.25	1.10
2	12	benzoic acid	80	UV-ozone	DMF	130	0.25	1.14
3	24	none	–	UV-ozone	DMF	130	0.1	1.00
4	24	none	–	UV-ozone	DMF	130	0.25	1.04
5	24	benzoic acid	40	UV-ozone	DMF	130	0.1	1.03
6	24	benzoic acid	40	UV-ozone	DMF	130	0.25	1.02
7	24	benzoic acid	80	UV-ozone	DMF	130	0 (dropcast)	1.01
8	24	benzoic acid	80	UV-ozone	DMF	130	0.1	1.40
9	24	benzoic acid	80	UV-ozone	DMF	130	0.25	1.36
10	24	benzoic acid	80	UV-ozone	DMF	130	0.5	1.28
11	24	benzoic acid	80	UV-ozone	DMF	110	0.1	1.25
12	24	benzoic acid	80	UV-ozone	DMF + 1 wt% water	130	0.1	1.40
13	24	benzoic acid	80	UV-ozone	DMF + 1 wt% water	130	0.25	1.38
14	24	benzoic acid	80	UV-ozone	methanol	60	0 (dropcast)	1.06
15	24	benzoic acid	80	UV-ozone	methanol	60	0.1	1.22
16	24	benzoic acid	80	UV-ozone	methanol	60	0.25	1.18
17	24	benzoic acid	80	SiOx	DMF	130	0.1	1.38
18	24	benzoic acid	80	SiOx	DMF	130	0.25	1.35
19	24	benzoic acid	80	PTS	DMF	130	0.25	1.43
20	24	acetic acid	80	UV-ozone	DMF	130	0.1	1.03
21	24	acetic acid	80	UV-ozone	DMF	130	0.25	1.17
22	24	acetic acid	80	UV-ozone	methanol	60	0.1	1.14
23	24	acetic acid	80	UV-ozone	methanol	60	0.25	1.14

Supplementary References

1. J. H. Cavka, S. Jakobsen, U. Olsbye, N. Guillou, C. Lamberti, S. Bordiga, K. P. Lillerud CCDC 733458: Experimental Crystal Structure Determination, 2014, DOI: 10.5517/ccsm6yj.