Supporting Information for Gel-Network Incorporation into Single-Crystals: Effects of Gel Structures and Crystal-Gel Interaction

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Supporting Figures:



Fig. S1 PXRD patterns of the crystals grown in silica and agarose gels. All the four crystals grown in two gels are consistent with the standard ones.



Fig. S2 TGA curves of KDP crystals grown in 0.2w/v% and 1 w/v% agarose gels. It is difficult to distinguish the decomposition of agarose from the dehydration of KDP.



Fig. S3 Characterization of the gel structure of agarose and silica gels: (a) A schematic representation of the replica method used to image the gel structures. Step 1: to expose the bottom surface of calcite grown at the flat surface of SAM (16-Mercaptohexadecanoic acid)-modified Au substrate. The as-grown calcite crystals at the SAM/gel interface are welloriented with a flat bottom face for imaging and the detailed crystallization method at the SAM/gel interface was previously reported in ref. 1. Step 2: to image the exposed bottom surface. The calcite crystal incorporated the gel and became a replica of the gel-network. (b, c) SEM images of the bottom surfaces of calcite grown from (b) an agarose gel (1 w/v%) and (c) a silica gel (concentration of sodium metasilicate pentahydrate 9.0 w/v%); (d, e) SEM images of the etched NaF crystals grown in (d) an agarose gel and (e) a silica gel. White arrows highlight the incorporated fibrous structure in NaF crystal grown in agarose gel.

Supporting Table:

Table S1 Unit cell dimensions of crystals grown in silica and agarose gels

	Silica gel	Agarose gel	Ref. (PDF cards)
NaF	(4.630(5), 4.630(7), 4.619(5);	(4.629(6), 4.637(8), 4.644(5);	(4.633, 4.633, 4.633;
	90.04(2), 90.08(3), 89.91(3))	89.97(3), 90.16(2), 90.03(3))	90.00, 90.00, 90.00)
			PDF-36-1455
NaCl	(5.645(5), 5.637(5), 5.641(8);	(5.664(6), 5.622(5), 5.638(8);	(5.640, 5.640, 5.640;
	89.98(2), 90.03(2), 90.00(3))	90.02(2), 89.77(4), 90.15(3))	90.00, 90.00, 90.00)
			PDF-05-0628
KBr	(6.582(7), 6.601(7), 6.588(6);	(6.604(8), 6.597(6), 6.596(5);	(6.597, 6.597, 6.597;
	89.91(3), 90.02(4), 90.00(4))	89.99(4), 89.98(2), 90.02(3))	90.00, 90.00, 90.00)
			PDF-04-0531
KDP	(7.459(6), 7.430(9), 6.990(7);	(7.463(5), 7.467(5), 6.945(7);	(7.463, 7.467, 6.945;
	89.22(5), 89.16(3), 90.26(4))	90.02(3), 90.08(4), 89.57(4))	90.02, 90.08, 89.57)
			PDF-35-0807

Reference:

1. H. Y. Li and L. A. Estroff, J Am Chem Soc, 2007, 129, 5480-5483.