

Investigation on the formation mechanism of twinned crystals of hypoxanthine-doped beta-phase anhydrous guanine microplatelets

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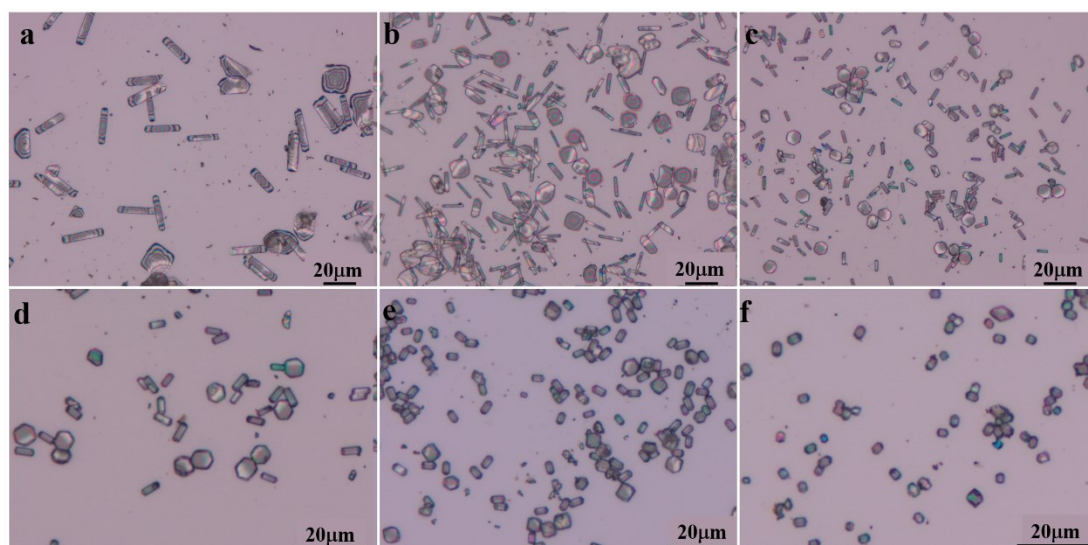


Figure S1. Light microscopy images of the synthesized I-doped AG crystals with different contents of hypoxanthine. (a) 0 mol%, (b) 11 mol%, (c) 18 mol%, (d) 24 mol%, (e) 26 mol%, (f) 29 mol%.

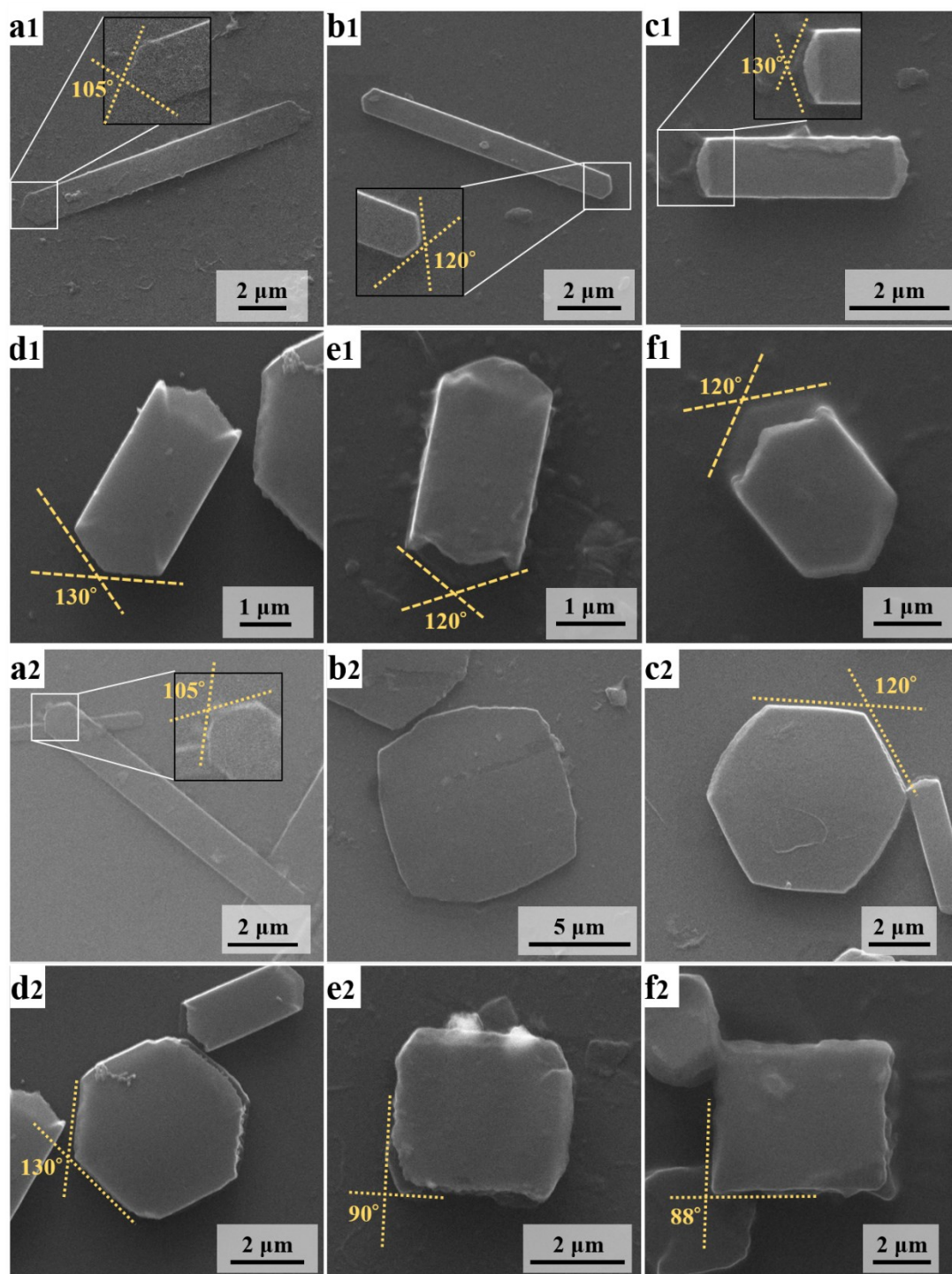


Figure S2. Zoomed-in SEM images for the of the synthesized I-doped AG crystals with different contents of hypoxanthine. (a₁, a₂) 0 mol%, (b₁, b₂) 11 mol%, (c₁, c₂) 18 mol%, (d₁, d₂) 24 mol%, (e₁, e₂) 26 mol%, (f₁, f₂) 29 mol%.

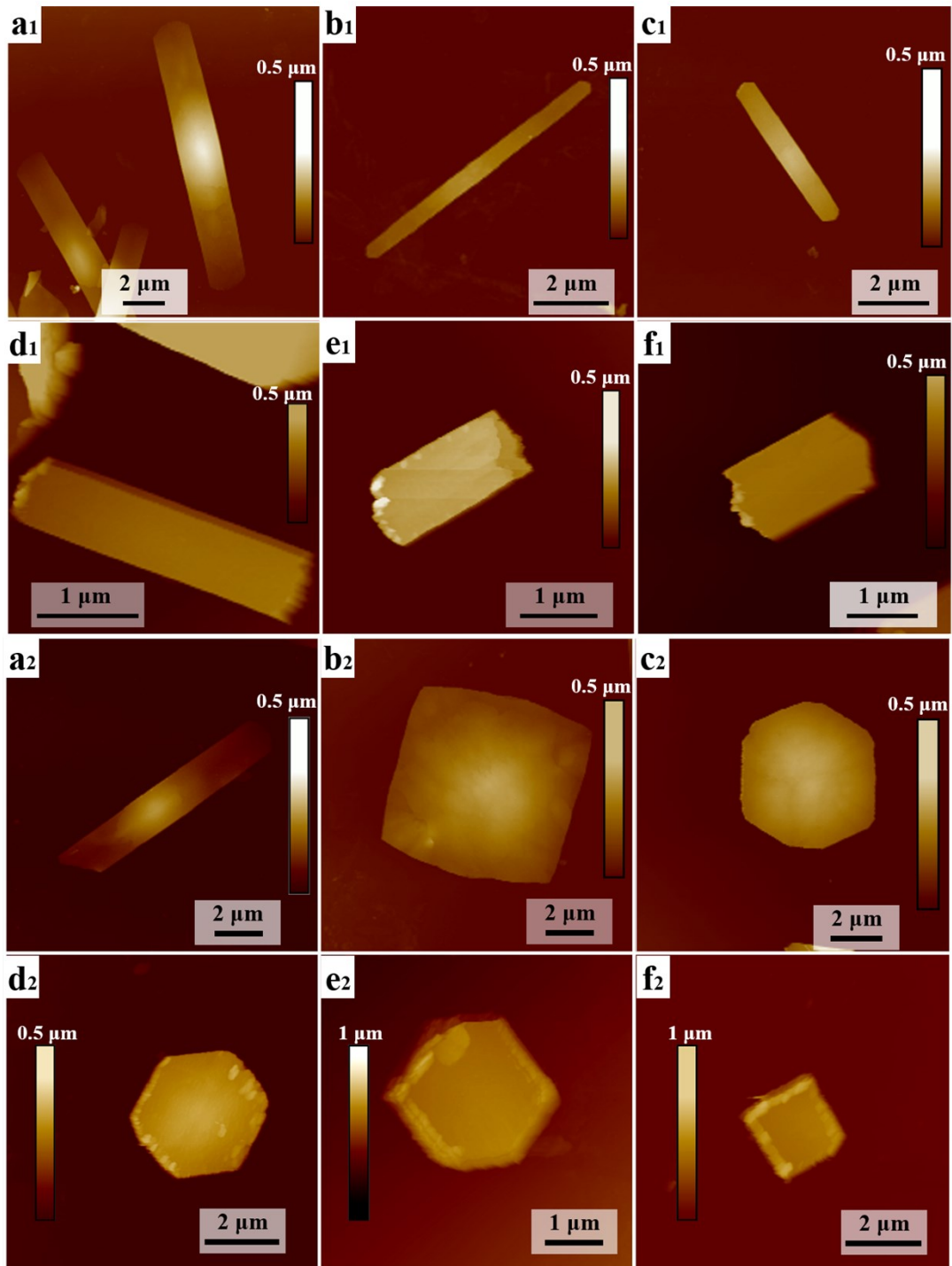


Figure S3. AFM characterizations of the synthesized I-doped AG crystals with different contents of hypoxanthine. (a₁, a₂) 0 mol%, (b₁, b₂) 11 mol%, (c₁, c₂) 18 mol%, (d₁, d₂) 24 mol%, (e₁, e₂) 26 mol%, (f₁, f₂) 29 mol%.

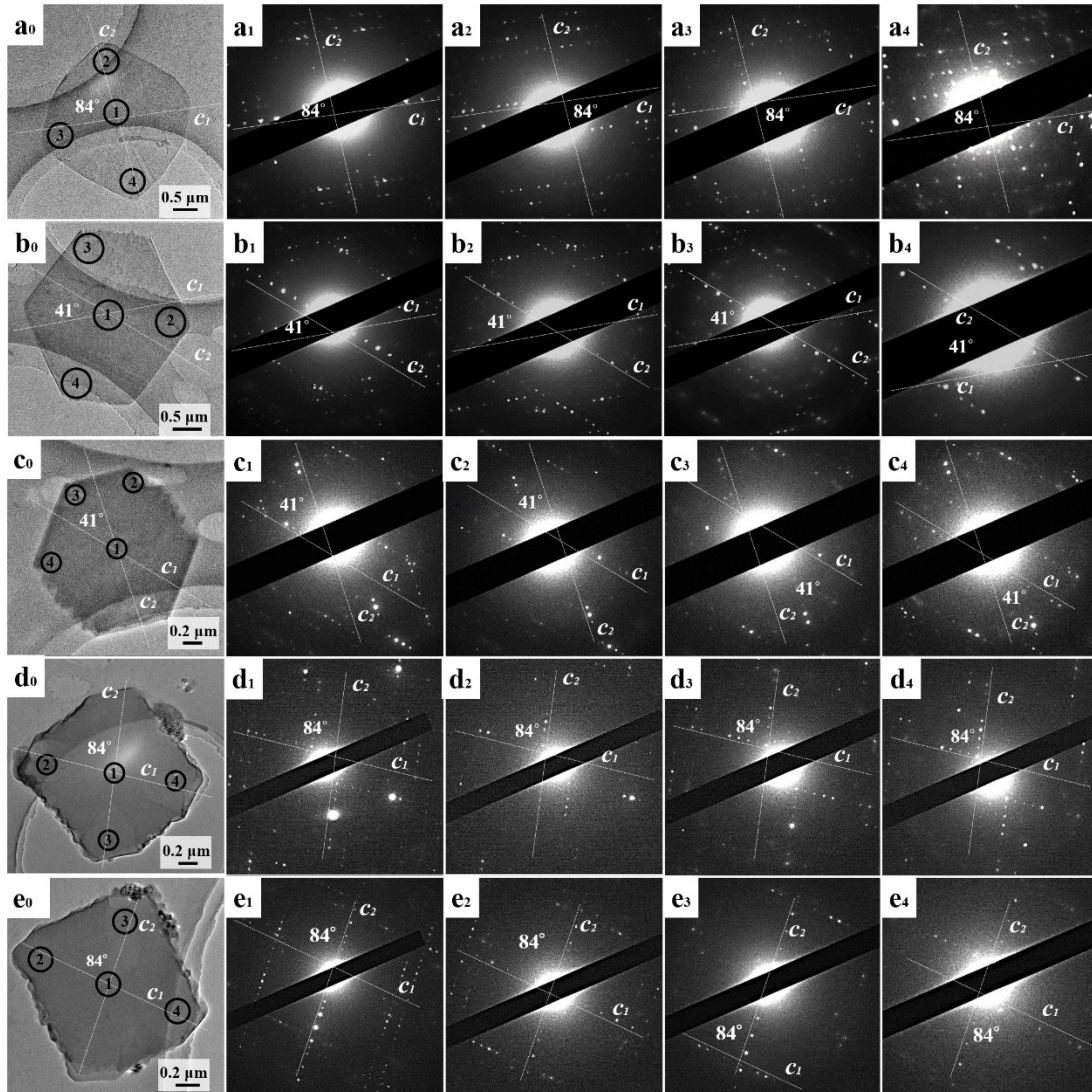


Figure S4. TEM images for the synthesized I-doped AG crystals with different contents of hypoxanthine and the SAED patterns collected from the different locations. (a_0 - a_5) 11 mol%, (b_0 - b_5) 18 mol%, (c_0 - c_5) 24 mol%, (d_0 - d_5) 26 mol%, (e_0 - e_5) 29 mol%. (a_0), (b_0), (c_0) and (d_0) TEM images. (a_1), (a_2), (a_3) and (a_4) SAED patterns of the ①, ②, ③ and ④ areas in the (a_0). (b_1), (b_2), (b_3) and (b_4) SAED patterns of the ①, ②, ③ and ④ areas in the (b_0). (c_1), (c_2), (c_3) and (c_4) SAED patterns of the ①, ②, ③ and ④ areas in the (c_0). (d_1), (d_2), (d_3) and (d_4) SAED patterns of the ①, ②, ③ and ④ areas in the (d_0). (e_1), (e_2), (e_3) and (e_4) SAED patterns of the ①, ②, ③ and ④ areas in the (e_0).

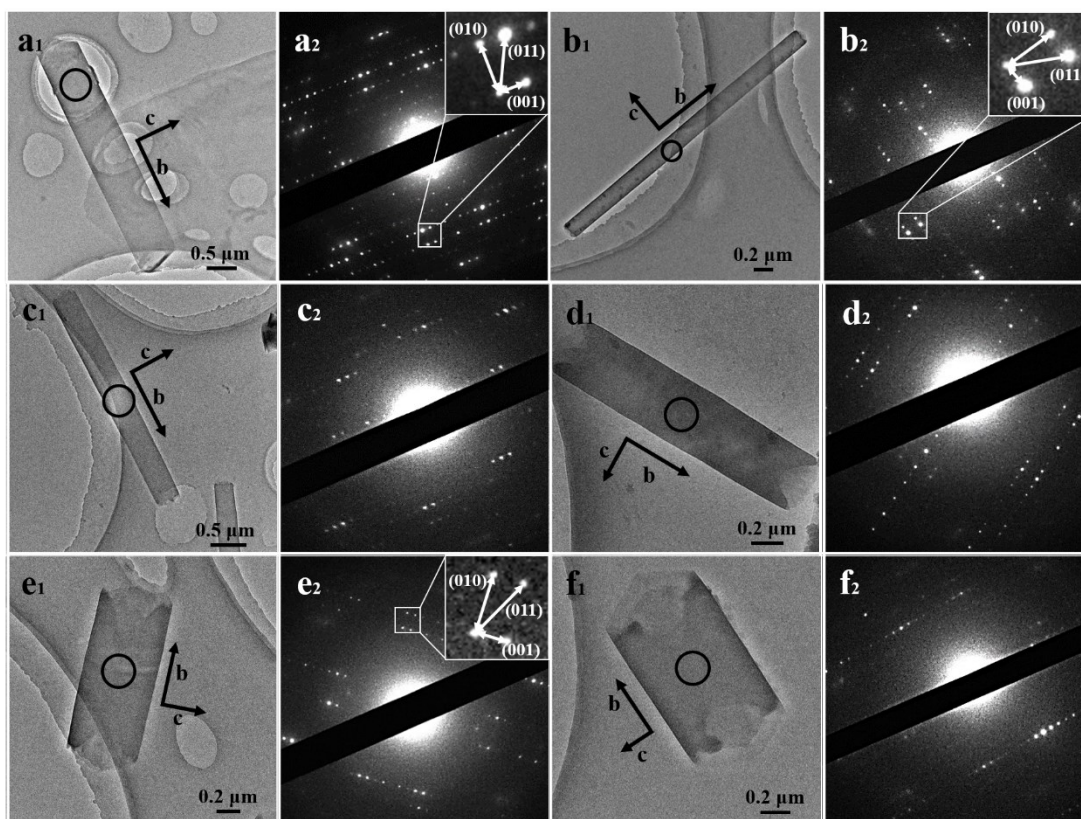


Figure S5. TEM images for the synthesized elongated-hexagon I-doped AG single crystals with different contents of hypoxanthine and their SAED patterns. (a₁, a₂) 0 mol%, (b₁, b₂) 11 mol%, (c₁, c₂) 18 mol%, (d₁, d₂) 24 mol%, (e₁, e₂) 26 mol%, (f₁, f₂) 29 mol%.

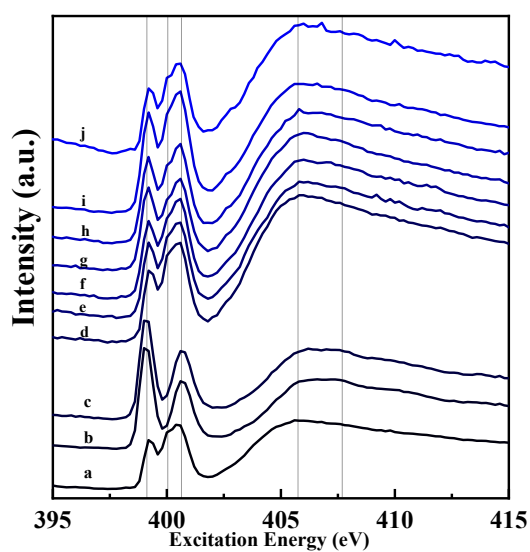


Figure S6. Nitrogen K-edge near edge X ray absorption fine structure spectra (NEXAFS) of the synthesized I-doped AG crystals with different contents of hypoxanthine. (a) I, (b) G, (c) mixed raw guanine and raw hypoxanthine with equal molar ratio, (d) 0 mol%, (e) 11 mol%, (f) 18 mol%, (g) 24 mol%, (h) 26 mol%, (i) 29 mol%, (j) Bio-G.

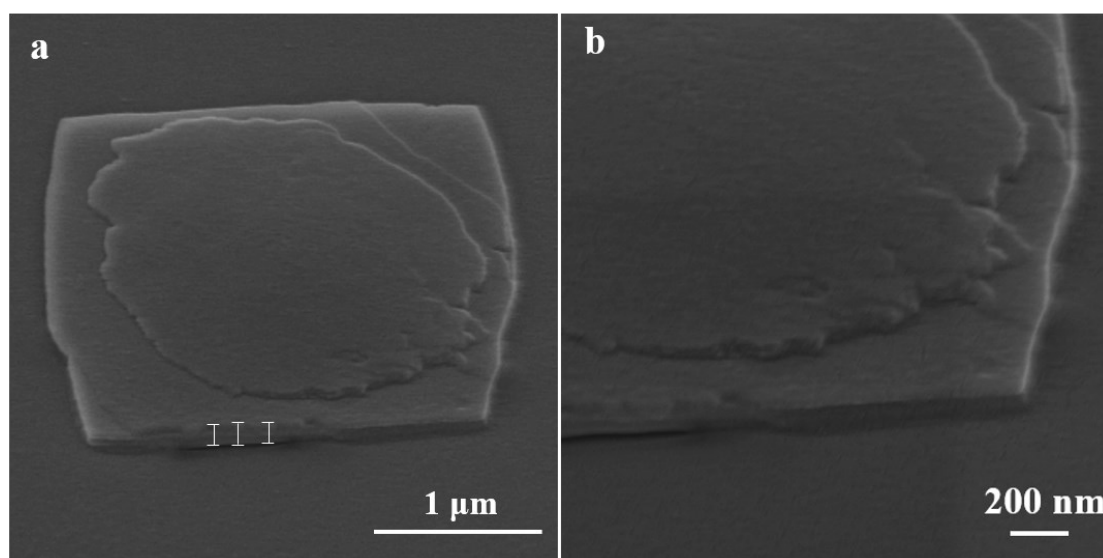


Figure S7. SEM images of the early stage of the I-doped β -AG crystals with 11 mol% of hypoxanthine formed with 1 hour crystallization time. (b) The zoom-in image of the edge of the (a). The sample holder was tilted 45° from the electron beam.

Table S1. HPLC for the synthesized I-doped AG crystals with different contents of hypoxanthine.

Sample name	Molar ratios of G and I in the reaction solutions	Mole of G (nM)	Mole of I (nM)	Mol% of I*
a	1:0	22477.6	12.5	0 mol%
b	1:1.5	32195.7	3919.3	11 mol%
c	1:3	8954.2	2000.5	18 mol %
d	1:4.5	8698.0	2770.1	24 mol %
e	1:6	7152.2	2531.4	26 mol %
f	1:7.5	21502.5	8666.8	29 mol %
g (Bio-hairtail)		3409600	29200	1 mol %
h (Bio-koi fish)		91300	13900	13 mol %

$$*\text{mol\% of I} = n(I)/(n(I) + n(G)) \times 100\%$$

Table S2. ¹³C SSNMR for the synthesized I-doped AG crystals with different contents of hypoxanthine.

Sample name	C6(G-I) (ppm)	C2(G) (ppm)	C4(G)	C2(I) (ppm)	C4(I) (ppm)	C8(G-I) (ppm)	C5(I) (ppm)	Unknown peak(ppm)	C5(G) (ppm)
I	159.2			149.5	145.4	141.9	122.5		
G	159.7	156.7	154.9			142.1			106.2
G/I*	159.5	156.8	154.9	149.7	145.4	142	122.5		106.2
a(0%)	160.1	157.1	155.4			141.9			106.7
b(11%)	160.6	157				141.9		115.7	107.3
c(18%)	160.5	157				142		115.2	107.2
d(24%)	160.3	156.9				141.7	121.7	114.9	107.2
e(26%)	160.1	156.9		149.6		142.3	121.6	114.9	107
f(28%)	160.2	157		149.4		142.8	121.8	115	107.3
Bio-G	160.2	157.6	156			142.4			107.3

* G mixed with 50 mol% of I.