

Supporting Information

II-VI Organic-Inorganic Hybrid Nanostructures with Greatly Enhanced Optoelectronic Properties, Perfectly Ordered Structures, and Over 15-Year Shelf Stability

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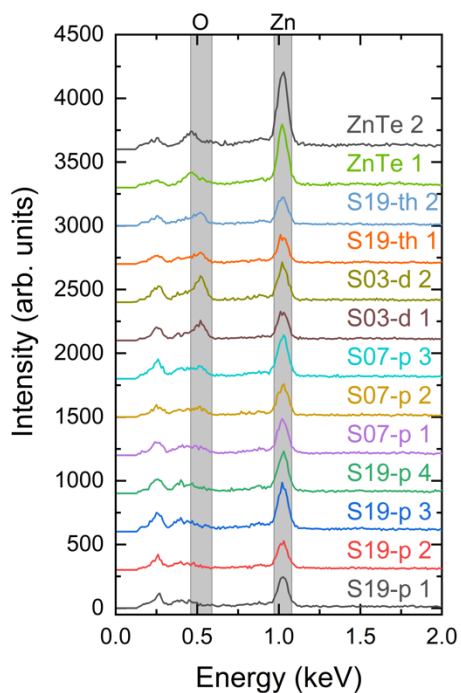
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Figure S1

a



b

	Mean	Std error
ZnTe	0.16	0.04
S19-p	0.05	0.02
S07-p	0.41	0.04
S03-d	1.08	0.07
S19-th	0.71	0.11

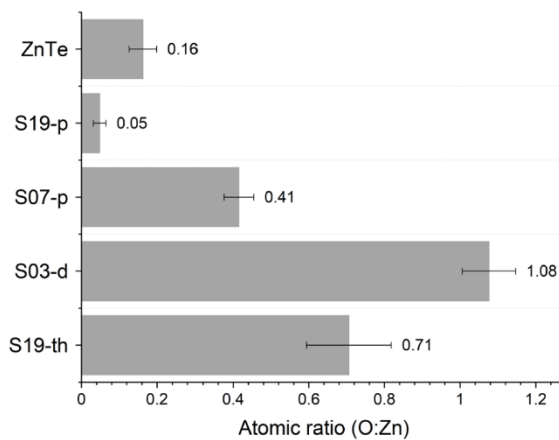


Figure S1. EDX and atomic ratio analysis. a) EDX spectra of different samples. b) Atomic ratios of O:Zn obtained from integrated peak intensities of EDX spectra.

Figure S2

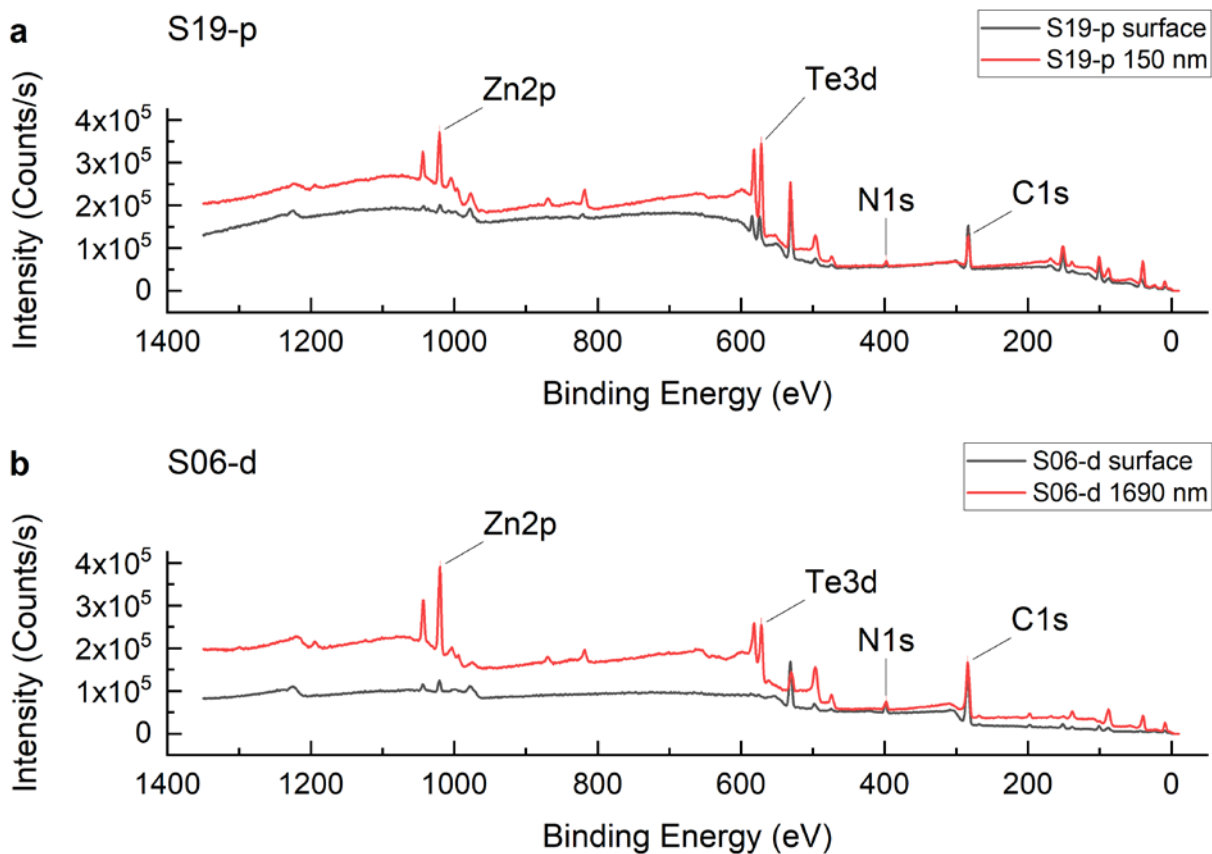


Figure S2. XPS spectra at different etching times or depths in an extended spectral range. a) a pristine sample S19-p, b) an optically degraded sample S06-d.

Figure S3

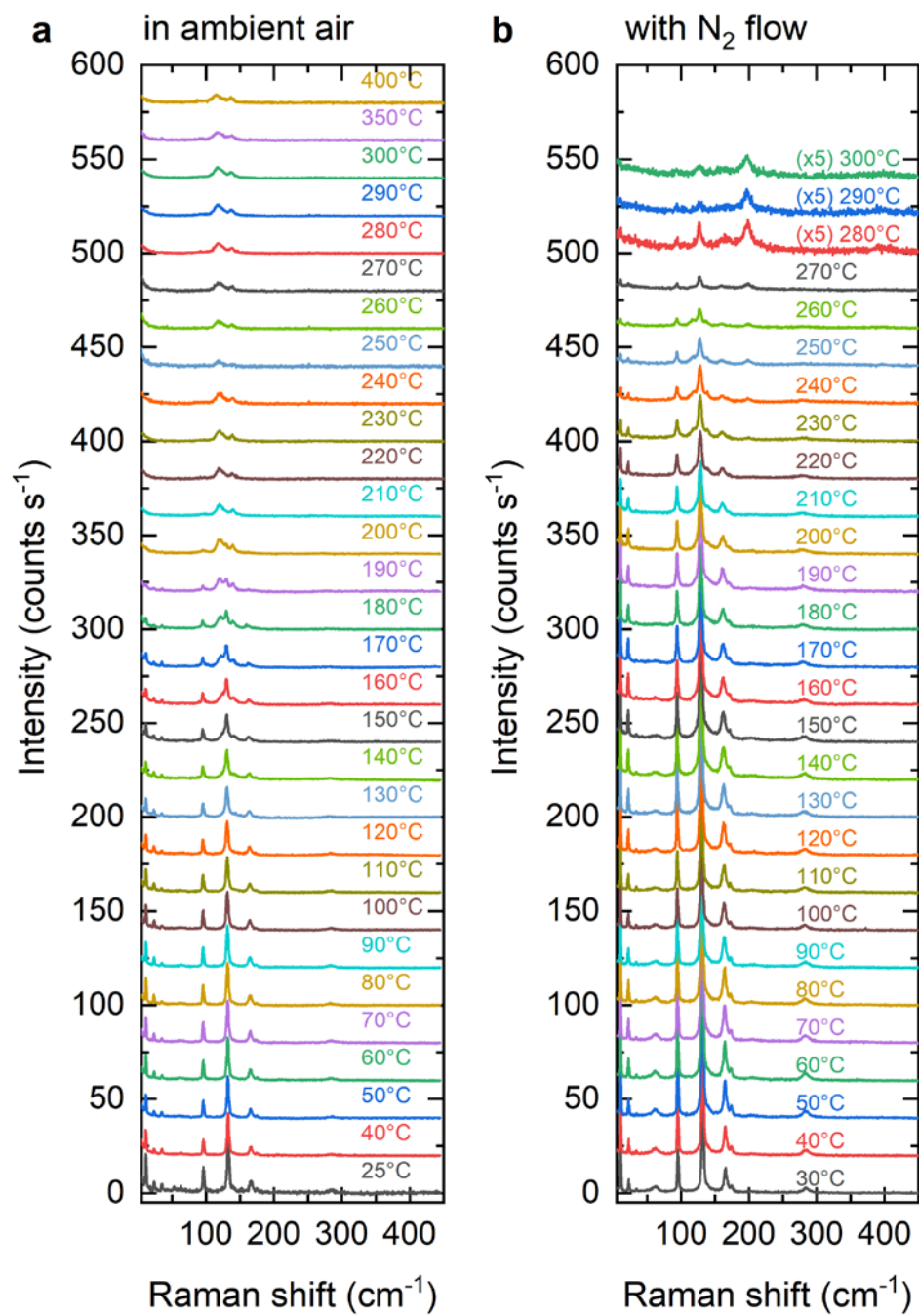
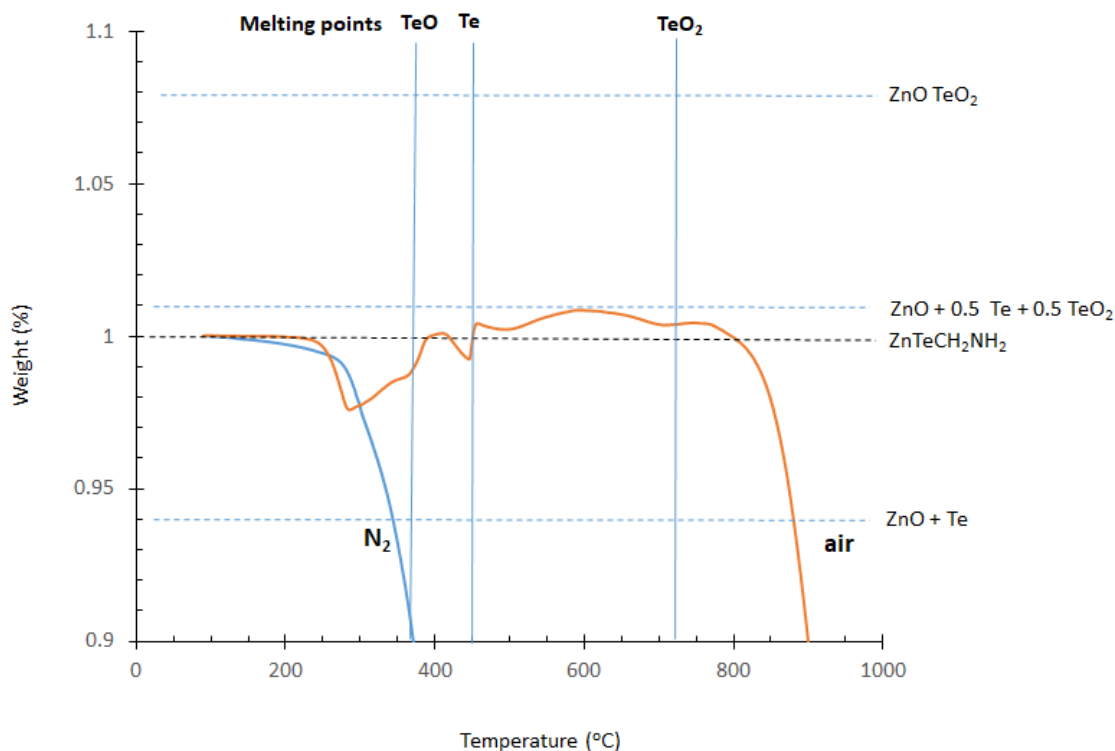


Figure S3. *In-situ* heating studies using Raman spectroscopy for a freshly made sample S19-p in air (a) and N₂ (b).

Figure S4



Formula	MW	Relative mass
ZnTe(CH ₂ NH ₂)	223.0296	1.00
ZnTeO ₃	240.9782	1.08
ZnTeO ₂	224.9788	1.01
ZnTeO	208.9794	0.94
ZnTe	192.98	0.87

Figure S4. Analyses of TGA curves for a freshly made sample S19-p in air and N₂. Horizontal lines indicate the masses of different potential degradation products, with the values show in the table below. The vertical lines indicate the melting temperatures for different Te products: 370, 450, and 720 °C for TeO, Te, and TeO₂, respectively [1].

[1] V.P. Itkin, C.B. Alcock, The O-Te (Oxygen-Tellurium) System, J Phase Equilib. 17 (1996) 533–538. doi:10.1007/bf02666000.

Figure S5

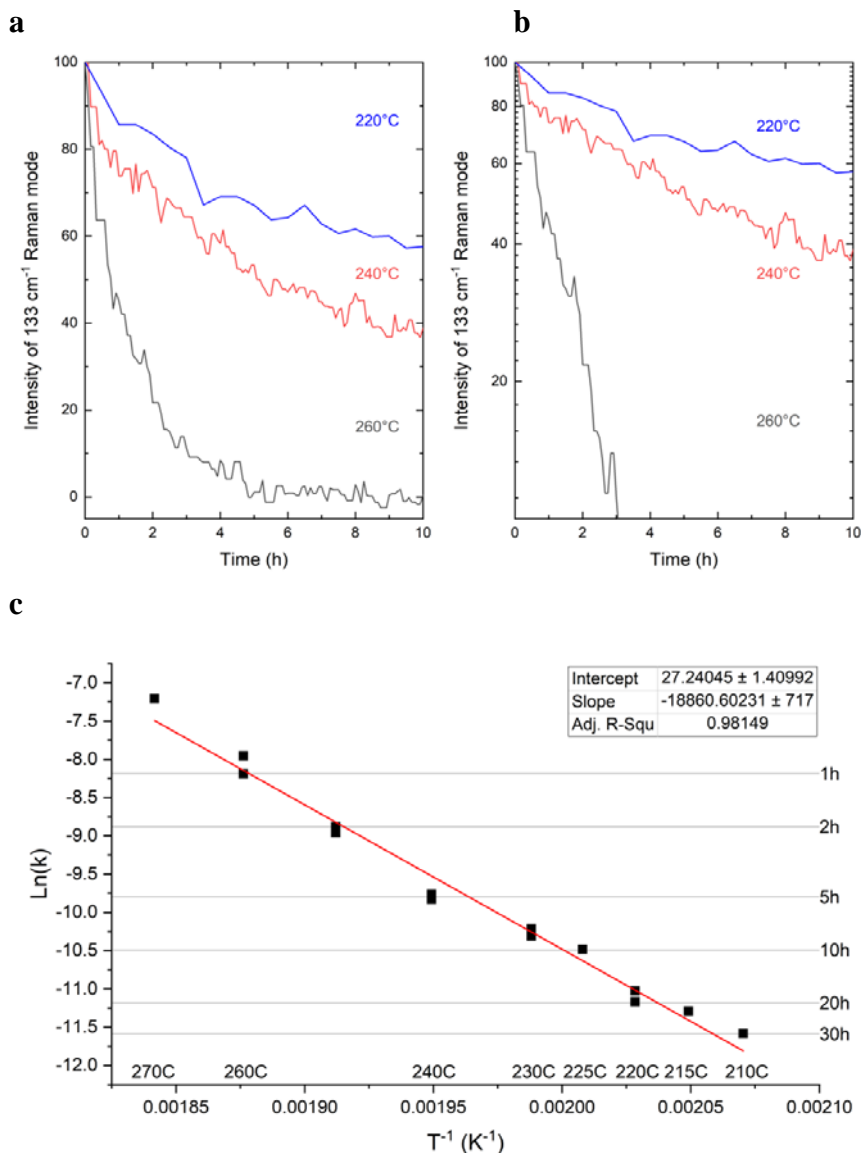


Figure S5. Use Arrhenius relationship $k = A\exp(-E_A/kT)$ to estimate activation energy E_A of thermal degradation by monitoring the intensity decay of the 133 cm⁻¹ Raman mode of the hybrid structure at different elevated temperatures in N₂. (a) and (b): peak intensity vs. time plots at selected temperatures in linear scale (a), and log scale (b). (c) Linear fit of Ln(k) vs. Temperature. The rate constant k at each temperature is determined by $1/t_{1/2}$, where $t_{1/2}$ is the intensity decay time of the 133 cm⁻¹ Raman mode reaching 50% of the $t = 0$ intensity. The fitting yielded a slope of 18860 ± 717 K, corresponding to an estimated $E_A = 1.63 \pm 0.06$ eV; and $\text{Ln}(A) = 27.24 \pm 1.41$, corresponding to $A = 6.8 (-5.1, +20.9) \times 10^{11} \text{ s}^{-1}$. Using the fitted line, the estimated $t_{1/2}(25^\circ\text{C}) = 1.44 \times 10^8$ years.

Table S1

Observed Raman mode frequencies and the corresponding calculated phonon mode frequencies and their symmetry assignments.

Figure	Observed frequency [cm ⁻¹]	Calculated phonon mode frequency [cm ⁻¹]	Symmetry	Corresponding en mode
1c	12.11	14.34	B2g	
1c	24.26	22.96	Ag	
1c	62.61			
1c	96.88	95.92	Ag	
1c	133.38	137.12	Ag	
1c	167.09	172.61	B2g	
1c	175.22	180.05	Ag	
1c	286.74	289.71	Ag	
1d	540.71	538.79	Ag	
1d	567.03	606.56	B2g	
1d	988.53	996.32	Ag	
1d	1170.35	1156.56	Ag	
1d	1596.71	1579.37	Ag	
1d	2868.82	2928.87	Ag	C-H vibration (2860 cm ⁻¹)
1d	2916.37	2965.59	B2g	C-H vibration (2928 cm ⁻¹)
1d	3128.44	3179.35	Ag	
1d	3203.68	3208.25	B2g	

Table S2

Powder diffraction analyses of a pristine sample S19-p and an optically degraded sample S06-d, yielding nearly identical (a , b , c) lattice constants.

	S19-p	S06-d	Ref. (24)	Ref. (27)
a (Å)	5.6709(9)	5.6736(6)	5.660(1)	5.6787(2)
b (Å)	17.160(3)	17.169(2)	17.156(3)	17.1998(6)
c (Å)	4.3403(6)	4.3445(5)	4.336(1)	4.3523(1)
α, β, γ	90°	90°	90°	90°
Volume (Å ³)	422.37(12)	423.21(9)	421.04(14)	425.10(4)
$R1$, <i>obs.</i>	0.0371	0.0365	0.0495	
$wR2$, <i>obs.</i>	0.0766	0.0896	0.0816	

Table S3

XRD (0,n,0) reflection peak relative intensities, normalized to (0,6,0). Simulated intensities were calculated from S19-p single-crystal structure data (using Mercury 3.10.2, CCDC).

h	k	l	S19-p	S07-p	S03-d	Simulated
0	2	0	84.2	119	27.2	75.1
0	4	0	5.72	10.4	8.02	7.02
0	6	0	100	100	100	100
0	8	0	59.6	59.4	57.4	63.7
0	10	0	5.72	7.29	5.56	6.82
0	12	0	7.69	9.38	3.7	6.41
0	14	0	18.3	14.6	4.94	16.3

Simulated XRD spectrum of (0,n,0) reflections:

