Supporting Information

Multifunctional Behavior of Molecules Comprising stacked Cytosine-Ag^{I}-Cytosine Base Pairs; Towards Conducting and Photoluminiscence DNA nanowires

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CONTENT

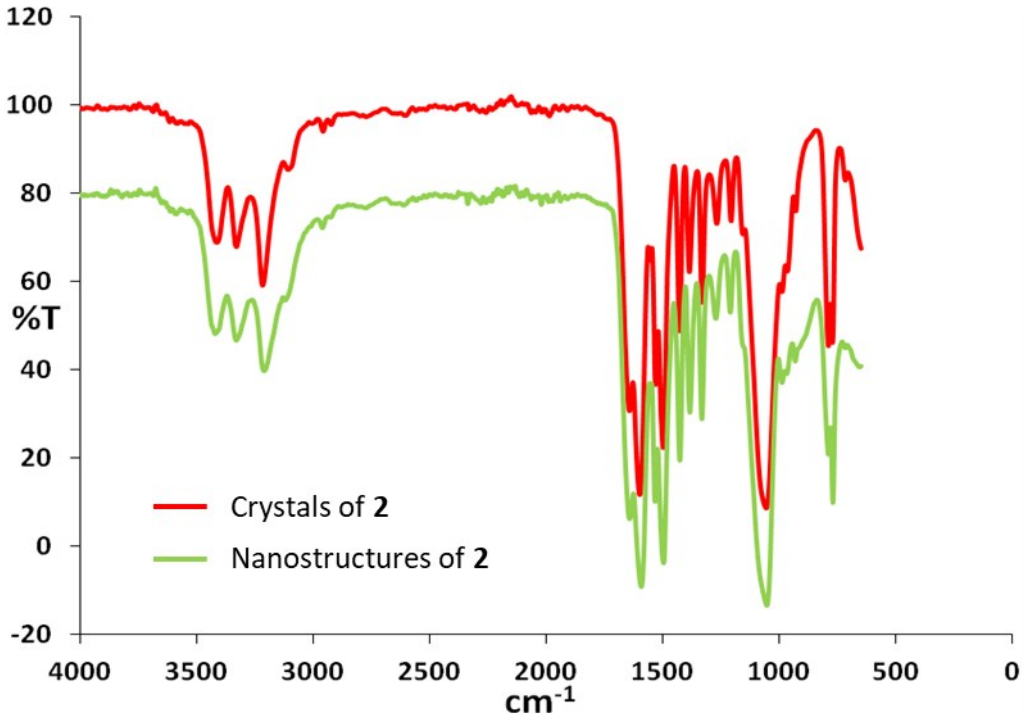

Figure S1. FTIR spectra for complex **2**: Crystal employed for single crystal X-ray diffraction studies (red line) and compound prepared on Si/SiO_2 wafers (green line).

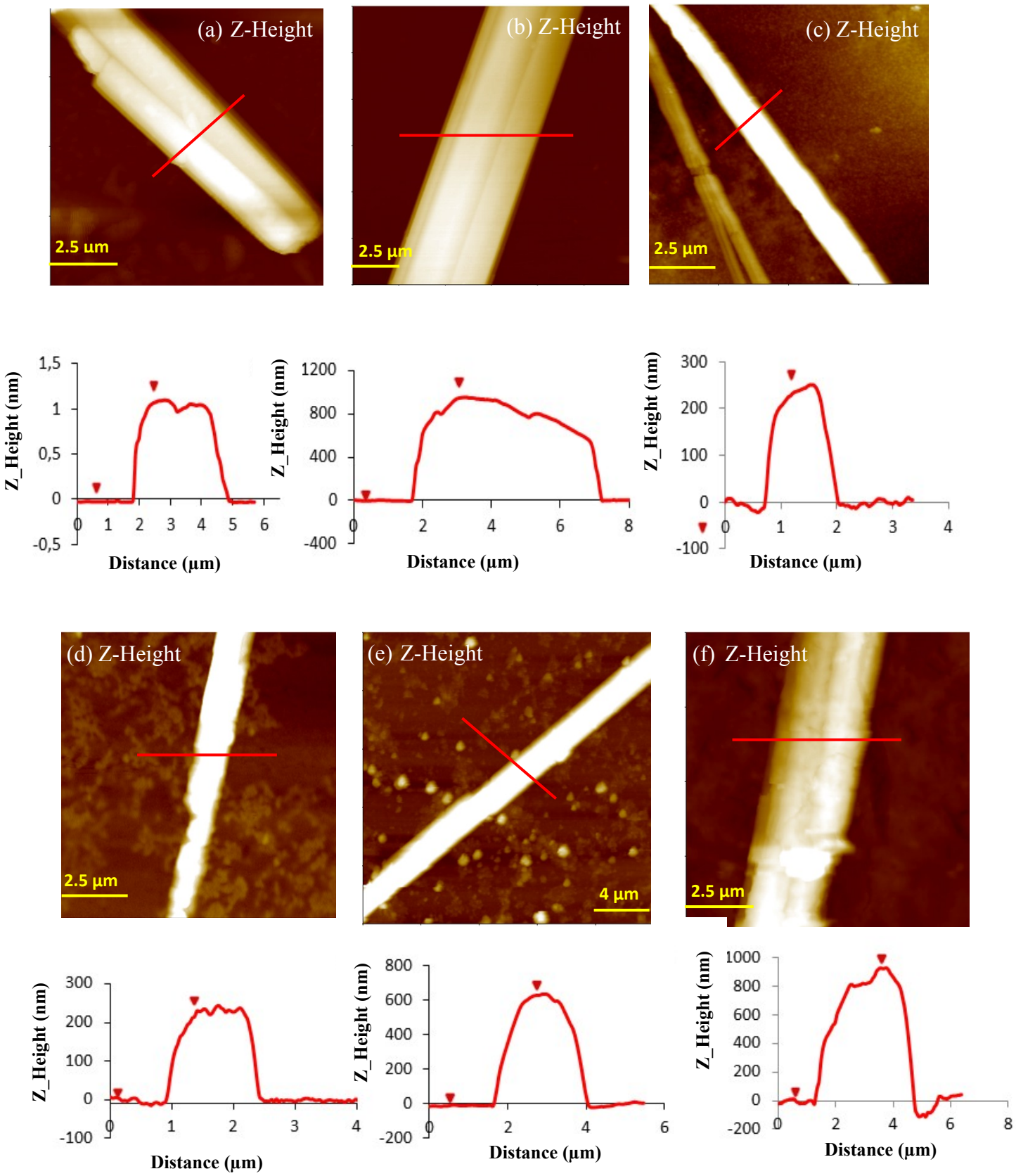

Figure S2. Z-Height Images and corresponding Z-Height Profiles for compound **2** on Si/SiO_2 wafers of repeated syntheses. (a) Z_Height is 1 µm, (b) Z Height 950 nm and (c) Z Height 250 nm, (d) Z Height 240 nm, (e) Z Height 600 nm and (f) Z Height 910 nm, respectively.

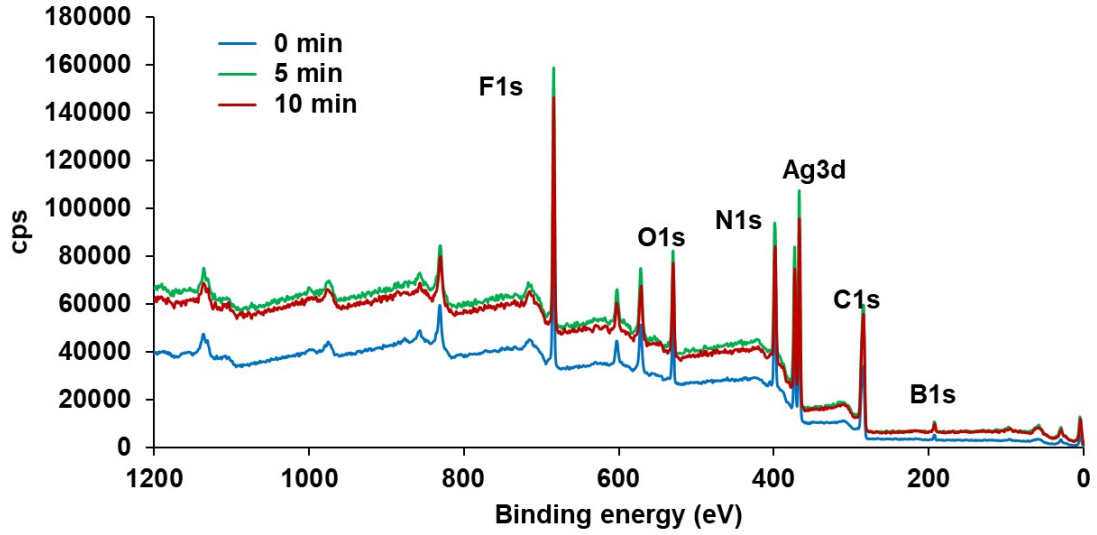

Figure S3. XPS survey spectra for complex **2** and **2H**, before and after exposure to hydrogen plasma, respectively. Blue Line corresponds to exposure time of 0 minutes to the cold hydrogen plasma (compound **2**); green line corresponds to 5 minutes and red line corresponds to 10 minutes (compound **2H**).

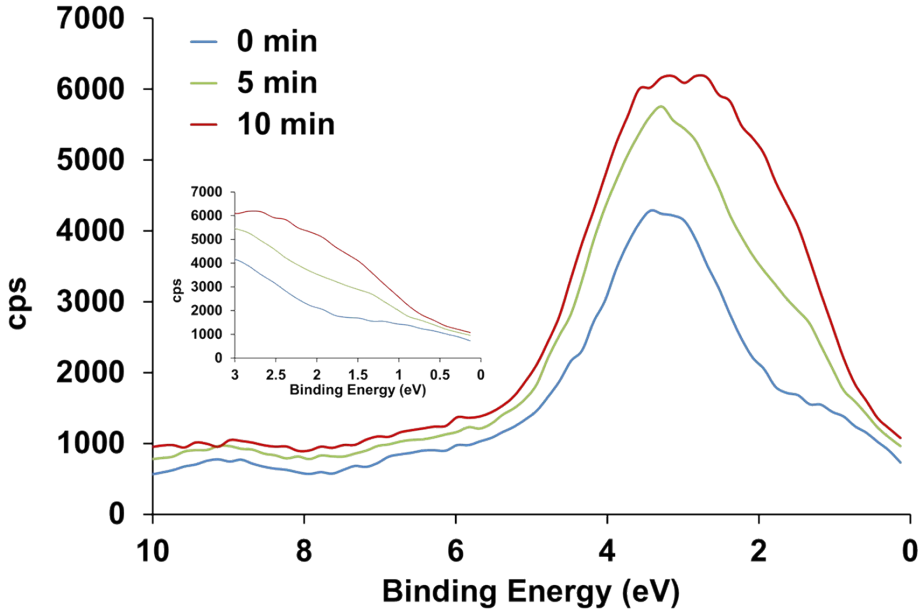

Figure S4. Valence band XPS spectra (inset is the enlarged region near the band edge) of **2**, before exposure to the hydrogen plasma (blue line) and after exposure for 5 min (green line) and 10 min (**2H**) (red line).

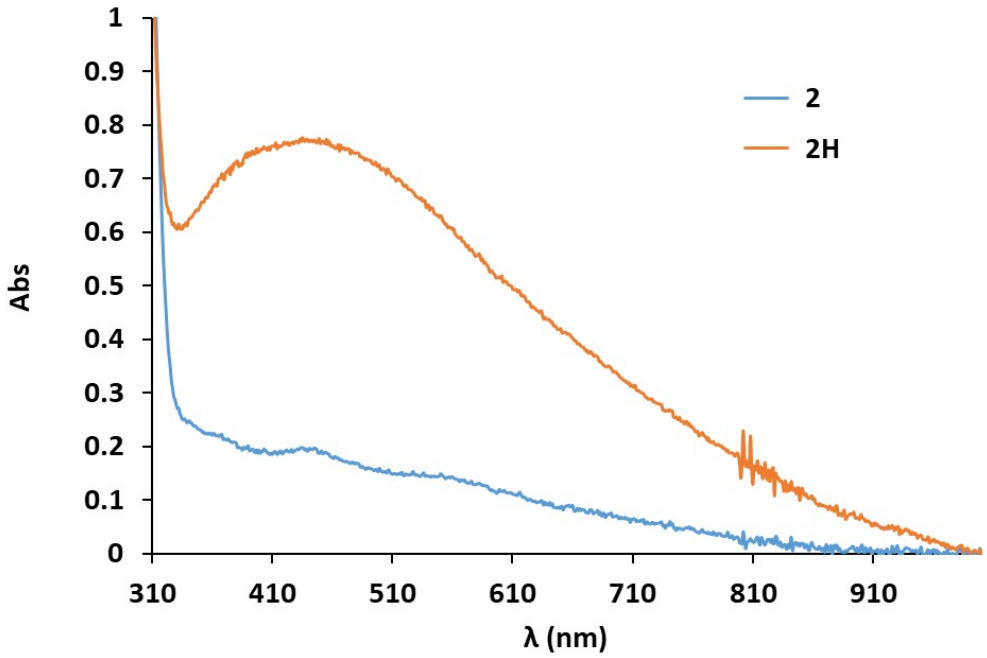

Figure S5. Solid-State UV-vis spectra for complex **2** (blue line) and **2H** (orange line)**,** before and after reduction treatment using hydrogen plasma, respectively.

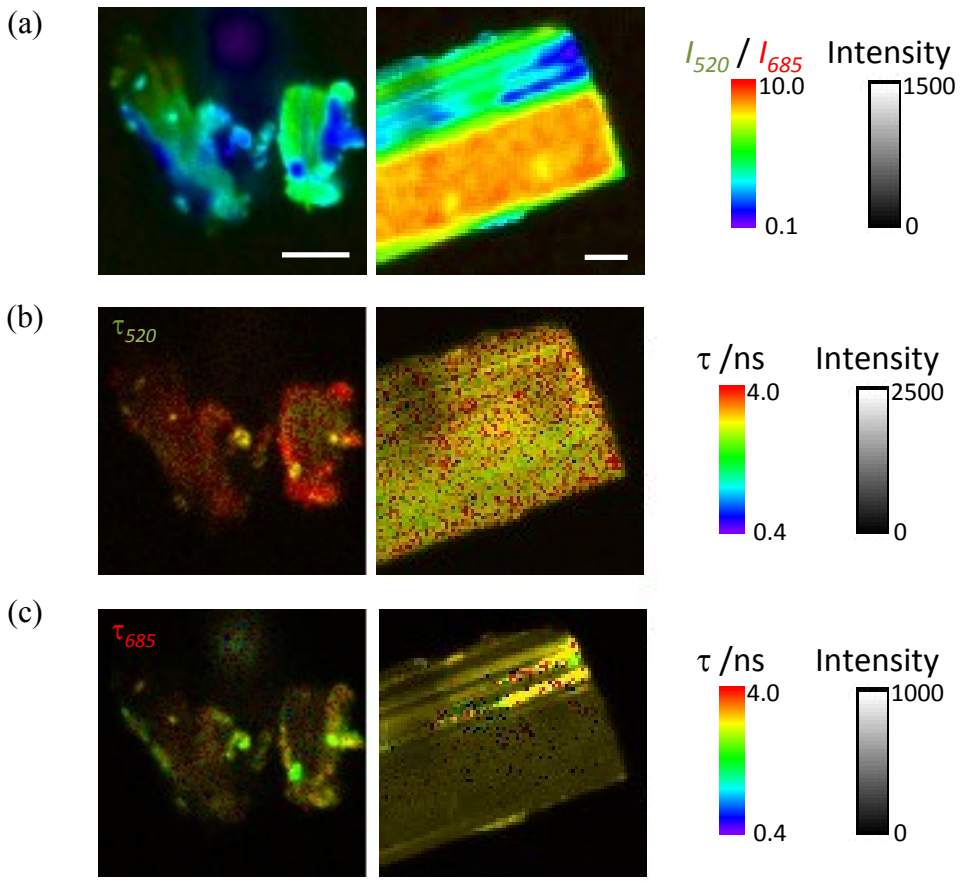

Figure S6. Multi-parametric PL emission imaging of **2H** crystals. (a) Intensity ratio imaging (I_{520}/I_{685}) on a pseudocolor scale between 0.1 and 10. (b) and (c) PL-FLIM imaging representing the long PL lifetime, τ, on the 520-nm channel (b) and the 685-nm channel (c). Scalebars represent 10 μm.

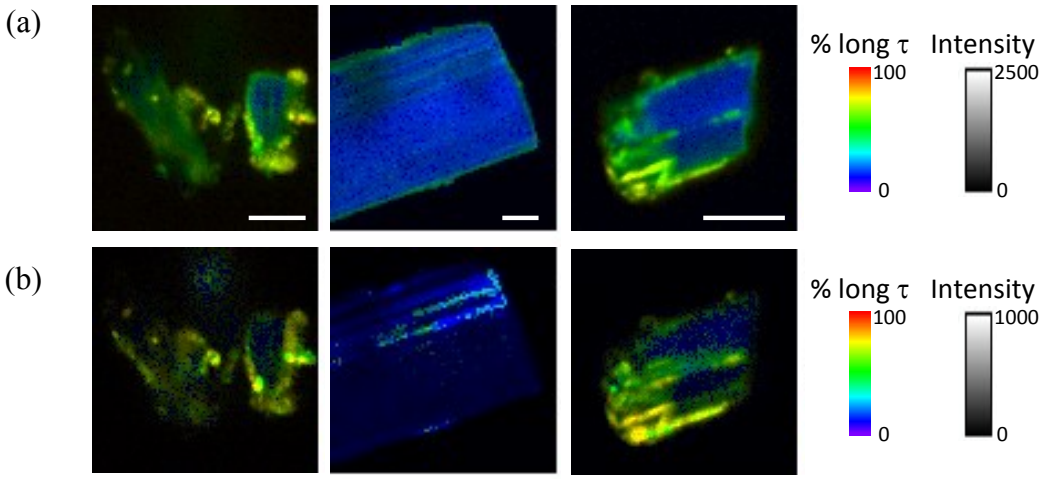

Figure S7. Multi-parametric PL emission imaging of **2H** crystals. Statistical weight of the long PL lifetime, τ, on the 520-nm channel (a) and the 685-nm channel (b) plotted on a pseudocolor scale from 0 to 100%. Scalebars represent 10 μm.

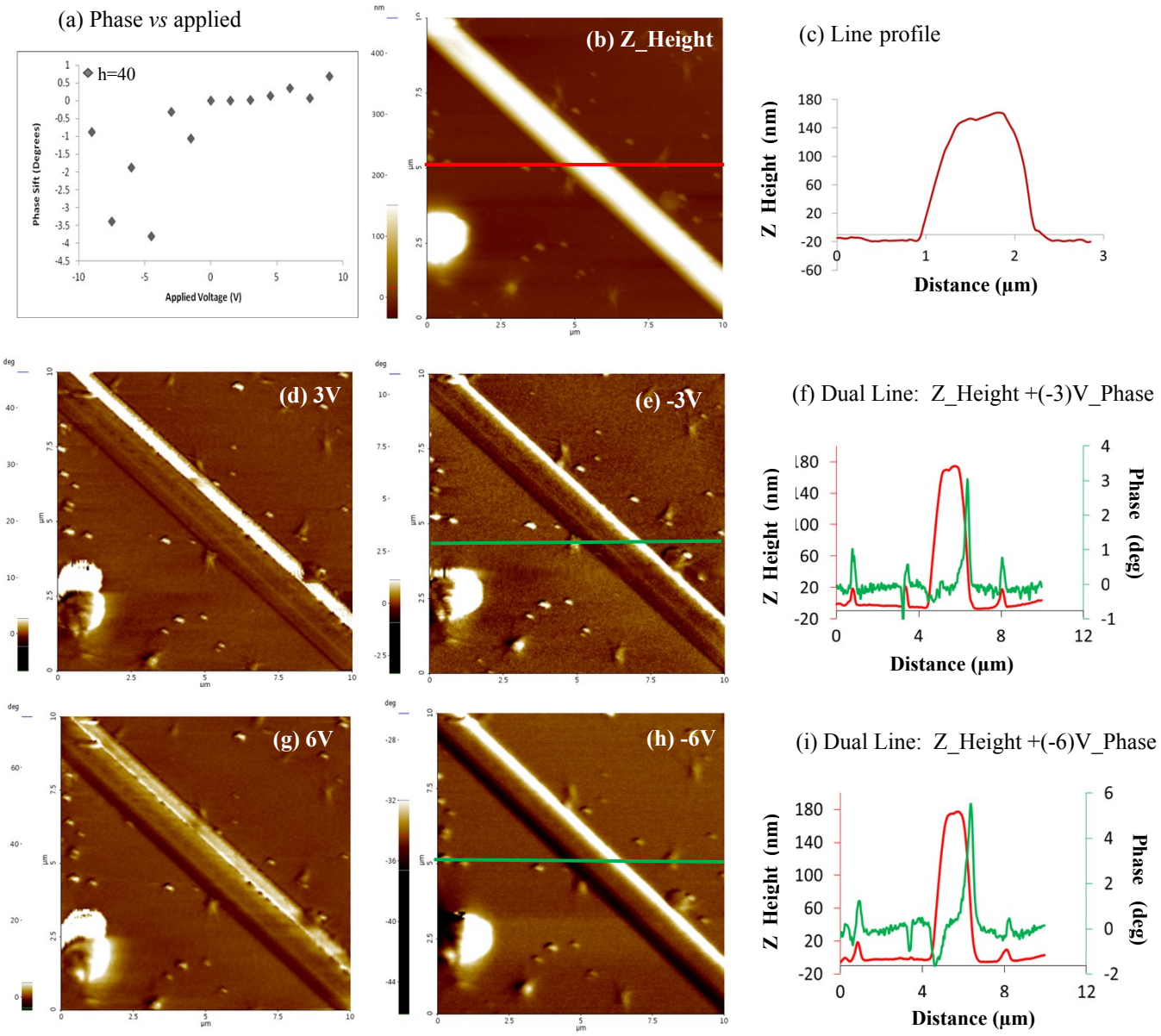

Figure S8. (a) Parabolic dependence of the phase shift vs bias voltages for **2** between -10 and +10 V; (b) Z_height image of the chain aligned on a SiO_2/Si surface. The size of scanned area is 10x10 µm; (c) Profile of the topography image. (d-i) EFM phase images at lift height 40 nm and tip/sample bias of (d) 3.0 V; (e) −3.0 V; (g) 6.0 V and (h) 6.0 V. (f) Line section through the phase image of the chain visible in this image at -3.0V. (i) Line section through the phase image of the chain visible in this image at -6.0V. The cantilever spring constant (k)=129.9 N•m^{-1} and the quality factor (Q)=274.

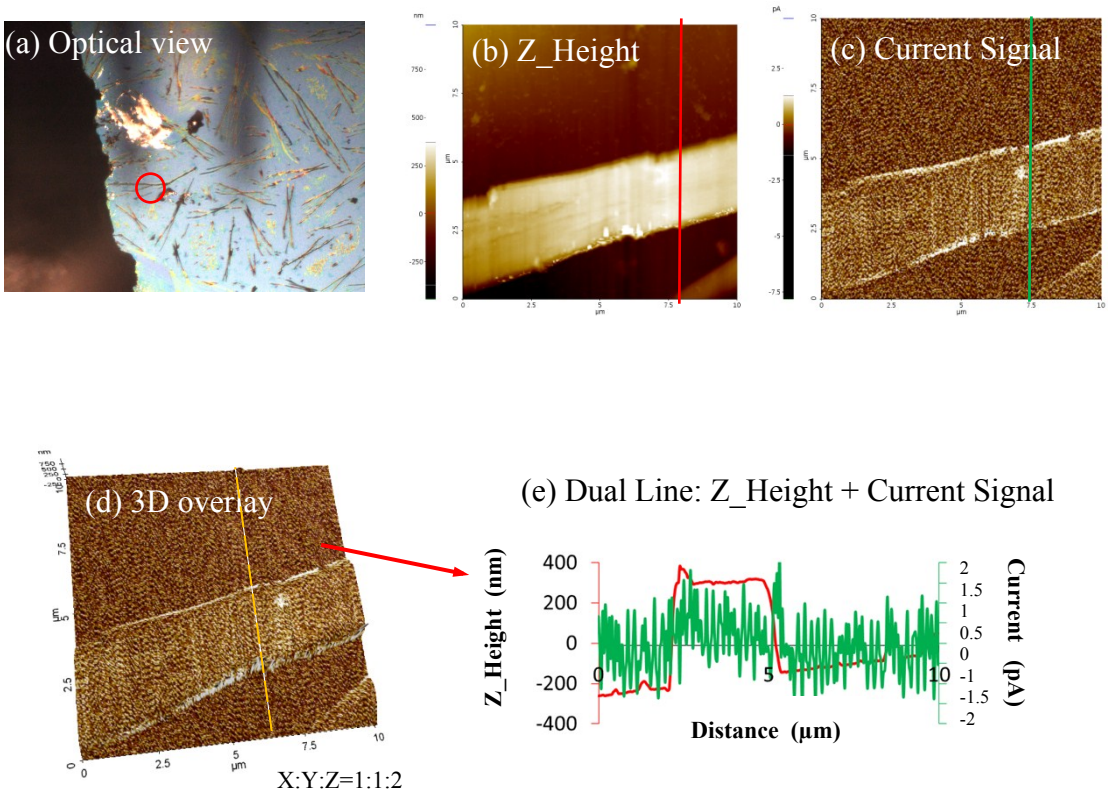

Figure S9. Crystals for **2** before reduction with cold hydrogen plasma. (a) Image from Optical Microscope structure: 384 x 288 µm protruding out from Ga/In Eutectic. Red circle indicates the selected zone for measurements. (b) Z-Height Image (10x10 µm). (c) Current signal (10x10 µm) with Sample BIAS +10V. (d) 3D overlay of (b) and (c). (e) Dual Line Profile for Z-Height and Current Signal.

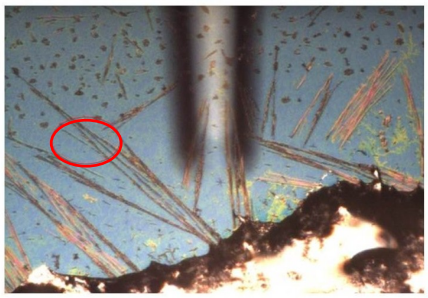

Figure S10. Image from Optical Microscope showing microcrystals of **2H** protruding out from Ga/In Eutectic. Red circle indicates the selected zone for measurements. Field of view: 384 x 288 µm.

Table S1. Crystallographic data and structure refinement details.

Compound	1	2	3
Chem. form.	$C_{100}H_{158}N_{70}O_{60}Ag_{10}$	$C_{80}H_{112}N_{48}O_{16}B_8F_{32}Ag_8$	$C_{80}H_{112}N_{48}O_{48}Cl_8Ag_8$
CCDC	1847831	1847832	1847833
Form. weight	4379.65	3559.61	3660.73
Cryst. system	Monoclinic	Orthorhombic	Orthorhombic
Space group	$P2_1/c$	$P2_12_12_1$	$P2_12_12_1$
a (Å)	25.5741(16)	21.7990(11)	21.9528(19)
b (Å)	26.2813(7)	22.6096(15)	22.8449(16)
c (Å)	24.8077(18)	26.0615(17)	26.174(2)
α (°)	90	90	90
β (°)	110.412(2)	90	90
γ (°)	90	90	90
V (Å^3)	15626.8(18)	12844.8(14)	13126.3(18)
Z	4	4	4
GOF [a]	1.016	1.010	1.095
R_{int}	0.2326	0.1077	0.1453
R_1 [b] / wR^2 [c] [I>2σ(I)]	0.0756 / 0.1662	0.0377 / 0.0670	0.0767 / 0.1857
R_1 [b] / wR^2 [c] (all data)	0.1623 / 0.2160	0.0516 / 0.0718	0.1115 / 0.2051

Table S2. Bond distances (Å) for compounds 1 - 3

1	2	3
Ag1 Ag2 2.923(2)	Ag1 Ag2 2.9786(16)	Ag1 Ag2 2.969(2)
Ag1 Ag7 2.948(2)	Ag1 Ag8 2.9107(16)	Ag1 Ag8 3.003(2)
Ag1 N1A 2.116(15)	Ag1 N1A 2.158(13)	Ag1 N1A 2.148(16)
Ag1 N1Z 2.191(16)	Ag1 N1B 2.186(12)	Ag1 N1B 2.178(16)
Ag2 Ag3 2.902(2)	Ag2 Ag3 2.9433(16)	Ag2 Ag3 2.908(2)
Ag2 N1I 2.180(14)	Ag2 N1C 2.190(12)	Ag2 N1C 2.143(17)
Ag2 N1K 2.181(16)	Ag2 N1D 2.186(12)	Ag2 N1D 2.131(17)
Ag3 Ag6 3.024(2)	Ag3 Ag4 2.9025(16)	Ag3 Ag4 2.899(2)
Ag3 N1D 2.154(17)	Ag3 N1E 2.173(12)	Ag3 N1E 2.15(2)
Ag3 N1O 2.163(16)	Ag3 N1F 2.157(12)	Ag3 N1F 2.166(15)
Ag4 Ag6 3.088(2)	Ag4 Ag5 2.9261(17)	Ag4 Ag5 2.940(2)
Ag4 Ag9 3.085(3)	Ag4 N1G 2.175(10)	Ag4 N1G 2.178(19)
Ag4 N1E 2.174(16)	Ag4 N1H 2.149(12)	Ag4 N1H 2.132(18)
Ag4 N1P 2.180(17)	Ag5 Ag6 2.9467(16)	Ag5 Ag6 2.911(2)
Ag5 Ag7 3.007(2)	Ag5 N1I 2.178(11)	Ag5 N1I 2.177(16)
Ag5 Ag8 3.034(2)	Ag5 N1J 2.188(12)	Ag5 N1J 2.189(17)
Ag5 N1S 2.145(18)	Ag6 Ag7 2.9195(17)	Ag6 Ag7 2.923(2)
Ag5 N1Y 2.136(16)	Ag6 N1K 2.193(12)	Ag6 N1K 2.170(17)
Ag6 N1C 2.118(16)	Ag6 N1L 2.184(12)	Ag6 N1L 2.169(19)
Ag6 N1G 2.147(16)	Ag7 Ag8 2.9120(17)	Ag7 Ag8 2.904(2)
Ag7 N1B 2.155(16)	Ag7 N1M 2.185(12)	Ag7 N1M 2.180(17)
Ag7 N1M 2.102(15)	Ag7 N1N 2.173(11)	Ag7 N1N 2.186(16)
Ag8 Ag10 3.004(3)	Ag8 N1O 2.200(11)	Ag8 N1O 2.18(2)
Ag8 N1R 2.142(16)	Ag8 N1P 2.206(10)	Ag8 N1P 2.142(17)
Ag8 N1T 2.144(16)		
Ag9 Ag10 2.988(3)		
Ag9 N1F 2.214(18)		
Ag9 N1J 2.185(19)		
Ag10 Ag9 2.988(3)		
Ag10 N1H 2.25(2)		
Ag10 N1V 2.185(18)		