Electronic Supplementary Information for

To which sites were thiols added? Insight on the thiol-yne click-based post-synthetic modification of conjugated microporous polymers

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Experimental Sections

SEM and TEM images were obtained by JSM7100F and JEOL2100F, respectively, at the Chiral Material Core Facility Center of Sungkyunkwan University. Solid state ^{13}C NMR spectra were obtained at CP/TOSS mode by a 500 MHz Bruker ADVANCE II NMR spectrometer at the NCIRF of Seoul National University. IR spectra were obtained by a Bruker VERTEX 70 FT-IR spectrometer. Elemental analysis was conducted by a CE EA1110 analyzer. The N_2 adsorption-desorption isotherm curves were obtained by a Micromeritics ASAP2020. Pore size distribution diagrams were obtained by the DFT method. Powder XRD patterns were obtained by a Rigaku MAX-2200. Solution state ^{1}H and ^{13}C NMR spectra were obtained by a 500 MHz Varian spectrometer. High-resolution mass spectra were obtained by a JEOL JMS 700.

Synthesis of H-CMP-1 and H-CMP-PT

For the use of templates, silica spheres with an average diameter of 200 nm and a surface area of 20 m^2/g were prepared by the Stöber method reported in the literature.[1] In this work, we applied the following synthetic procedures. Ethanol (200 mL), distilled water (8 mL), and ammonia solution (28% in water, 5 mL) were added to a 250 mL round bottomed flask. After stirring at room temperature for 30 min, tetraethyl orthosilicate (TEOS, 14 mL, 63 mmol) was added to the reaction mixture. After stirring at room temperature for 18 h, the reaction mixture was transferred to an Erlenmeyer flask. After adding hexane (200 mL) and methylene chloride (30 mL), the aggregated silica spheres were separated by centrifugation, washed with a mixture of methanol (20 mL) and acetone (20 mL) four times, and dried under vacuum.

For the preparation of SiO_2@CMP-1, silica spheres (0.60 g), $(PPh_3)_2PdCl_2$ (28 mg, 40 μmol), and CuI (7.6 mg, 40 μmol) were added to a flame-dried Schlenk flask under argon. After distilled toluene (20 mL) and distilled triethylamine (40 mL) were added, the reaction mixture was sonicated at room temperature for 1 h under argon. After 1,3,5-triethynylbenzene (60 mg, 0.40 mmol) and 1,4-diiodobenzene (0.198 mg, 0.600 mmol) were added, the reaction mixture was stirred at 90°C for 12 h under argon. After being cooled to room temperature, solid (SiO_2@CMP-1) was separated by centrifugation, washed with a mixture of methylene chloride (15 mL), methanol (15 mL), and acetone (15 mL) five times, and dried under vacuum. For the preparation of H-CMP-1,

SiO_2@CMP-1 was added to a mixture of aqueous HF solution (48~51% in water, 7.5 mL), methanol (20 mL), and water (15 mL) in a 50 mL Falcon tube. After the reaction mixture was stirred at room temperature for 2 h, the solid (H-CMP-1) was separated by centrifugation, washed with a mixture of methanol (20 mL) and water (20 mL) five times and acetone (40 mL) three times, and dried under vacuum. *Caution: HF solution is extremely dangerous and toxic and thus, should be handled with specific gloves in a hood. After reaction, the excess HF solution should be quenched with NaOH solution.*

For the preparation of H-CMP-1-PT, H-CMP-1 (50 mg), azobis(isobutyronitrile) (AIBN, 0.43 g, 2.6 mmol), 1-propanethiol (0.24 mL, 2.6 mmol), and distilled toluene (16 mL) were added to a flame-dried Schlenk flask. The reaction mixture was stirred at 90°C for 24 h. After being cooled to room temperature, the solid (H-CMP-1-PT) was separated by centrifugation, washed with a mixture of methylene chloride (15 mL), methanol (15 mL), and acetone (15 mL) five times, and dried under vacuum.

Synthesis of H-CMP-Br and H-CMP-Br-PT

For the synthesis of H-CMP-Br, the same synthetic procedures used for the H-CMP-1 were applied, except using 1,3,5-triethynylbenzene (60 mg, 0.40 mmol) and 1,4-dibromobenzene (94 mg, 0.40 mmol), instead of 1,3,5-triethynylbenzene (60 mg, 0.40 mmol) and 1,4-diiodobenzene (0.198 mg, 0.600 mmol). The other procedures are the same as those for H-CMP-1. For the synthesis of H-CMP-Br-PT, the same synthetic procedures used for the H-CMP-1-PT were applied, except using H-CMP-Br (50 mg), instead of H-CMP-1 (50 mg). The other procedures are the same as those for H-CMP-1-PT.

Synthesis of H-CMP-G and H-CMP-G-PT

For the synthesis of H-CMP-G, the same synthetic procedures used for the H-CMP-1 were applied, except using 1,3,5-triethynylbenzene (60 mg, 0.40 mmol), instead of 1,3,5-triethynylbenzene (60 mg, 0.40 mmol) and 1,4-diiodobenzene (0.198 mg, 0.600 mmol). The other procedures are the same as those for H-CMP-1. For the synthesis of H-CMP-G-PT, the same synthetic procedures used for the H-CMP-1-PT were applied, except using H-CMP-G (50 mg), instead of H-CMP-1 (50 mg). The other procedures are the same as those for H-CMP-1-PT.

Experimental procedures of model studies

For the single addition reaction[2] of 1-propanethiol to 1,2-diphenylacetylene, the same synthetic procedures used for the single addition reaction of 1-propanethiol to 1,4-diphenylbutadiyne were applied except using 1,2-diphenylacetylene instead of 1,4-diphenylbutadiyne (vide infra). The products are known compounds and their NMR spectra matched well with those in the literature.[2] Characterization data of (1,2-diphenylvinyl)(propyl)sulfane: Isolated yield: 87% (*Z*:*E*=57:43), a Z isomer, ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.1 Hz, 2H), 7.59 (d, *J* = 8.3 Hz, 2H), 7.42~7.03 (m, 6H), 6.79 (s, 1H), 2.39 (t, *J* = 7.3 Hz, 2H), 1.44 (sextet, 7.3 Hz, 2H), 0.81 (t, *J* = 7.3 Hz, 3H) ppm, an E isomer ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42~7.03 (m, 8H), 6.92 (d, *J* = 7.8 Hz, 2H), 6.73 (s, 1H), 2.51 (t, *J* = 7.3 Hz, 2H), 1.60 (sextet, 7.3 Hz, 2H), 0.96 (d, *J* = 7.3

Hz, 3H) ppm, ^{13}C NMR (125 MHz, $CDCl_3$) δ = 141.3, 138.4, 138.2, 137.9, 137.2, 136.9, 132.0, 129.7, 129.6, 128.9, 128.6, 128.4, 128.3, 128.0, 127.8, 127.1, 126.7, 126.4, 34.8, 33.9, 23.2, 22.6, 13.4, 13.2 ppm.

For the possible coupling of bromobenzene with 1-propanethiol in the presence of $(PPh_3)_2PdCl_2$ and CuI, bromobenzene (0.14 mL, 1.0 mmol), azobis(isobutyronitrile) (AIBN, 0.164 mg, 1.00 mmol), 1-propanethiol (0.093 mL, 1.0 mmol), and distilled toluene (2 mL) were added to a flame-dried Schlenk flask. The reaction mixture was stirred at 90°C for 24 h. After being cooled to room temperature, the solvent was evaporated by a rotary evaporator. The reaction mixture was analyzed by ^{1}H NMR spectroscopy, showing no reaction of bromobenzene. When the possible coupling of bromobenzene with 1-propanethiol was conducted in the absence of $(PPh_3)_2PdCl_2$ and CuI, no reaction was observed. When we used iodobenzene, instead of bromobenzene, no reactions were observed in the presence and absence of $(PPh_3)_2PdCl_2$ and CuI.

For the double addition reaction[3] of 1-propanethiol to 1,4-diphenylbutadiyne, 1,4-diphenylbutadiyne (0.20 g, 1.0 mmol), azobis(isobutyronitrile) (AIBN, 0.657 mg, 4.00 mmol), 1-propanethiol (0.37 mL, 4.0 mmol), and distilled toluene (20ml) were added to a flame-dried flask. The reaction mixture was stirred at 90°C for 24 h. After being cooled to room temperature, the product was extracted using methylene chloride and NH_4Cl aqueous solution. After drying the methylene chloride solution with $MgSO_4$, the solvent was evaporated by a rotary evaporator. The product was separated by flash column chromatography. Characterization data of (1*Z*,3*Z*)-1,4-diphenyl-1,4-bis(propylthio)buta-1,3-diene: Isolated yield: 53%, ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.63 (d, *J* = 7.4 Hz, 4H), 7.38 (t, *J* = 7.5 Hz, 4H), 7.35 (s, 2H), 7.31 (t, *J* = 7.3 Hz, 2H), 2.43 (t, *J* = 7.2 Hz, 4H), 1.45 (sextet, *J* = 7.3 Hz, 4H), 0.87 (t, *J* = 7.3 Hz, 6H) ppm, ^{13}C NMR (125 MHz, $CDCl_3$) δ = 140.3, 139.7, 131.2, 128.4, 128.1, 128.0, 34.9, 23.2, 13.2 ppm, HR-MS: Calc. $[M]^+$, $C_{22}H_{26}S_2$, 354.1476, Obs. 354.1473.

For the single addition reaction[4] of 1-propanethiol to 1,4-diphenylbutadiyne, the same synthetic procedures used for the double addition reaction of 1-propanethiol to 1,4-diphenylbutadiyne were applied except using azobis(isobutyronitrile) (AIBN, 0.164 mg, 1.00 mmol) and 1-propanethiol (0.093 mL, 1.0 mmol), instead of azobis(isobutyronitrile) (AIBN, 0.657 mg, 4.00 mmol) and 1-propanethiol (0.37 mL, 4.0 mmol). The other procedures are the same as those for the double 1-propanethiol adduct of 1,4-diphenylbutadiyne. Characterization data of (1,4-diphenylbut-1-en-3-yn-1-yl)(propyl)sulfane: Isolated yield: 27% (*Z*:*E*=60:40), a Z isomer, ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71~7.50 (m, 4H), 7.43~7.30 (m, 6H), 6.04 (s, 1H), 2.61 (t, *J* = 7.2 Hz, 2H), 1.51 (sextet, *J* = 7.3 Hz, 2H), 0.92 (t, *J* = 7.3 Hz, 3H) ppm, an E isomer ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71~7.49 (m, 4H), 7.49~7.28 (m, 6H), 5.88 (s, 1H), 2.66 (t, *J* = 7.2 Hz, 2H), 1.65 (sextet, *J* = 7.3 Hz, 2H), 0.99 (t, *J* = 7.4 Hz, 3H) ppm, ^{13}C NMR (125 MHz, $CDCl_3$) δ = 149.9, 139.0, 131.5, 131.2, 129.2, 129.1, 129.0, 128.8, 128.7, 128.5, 128.4, 128.3, 128.2, 128.1, 128.0, 127.9, 127.7, 127.3, 125.6, 123.7, 109.8, 103.9, 97.2, 87.7, 34.8, 34.5, 23.2, 22.1, 13.4, 13.1 ppm, HR-MS: Calc. $[M]^+$, $C_{19}H_{18}S$, 278.1129, Obs. 278.1130.

Computational simulations of strain energies for the PSM of CMPs

To investigate the reason for the different reactivities of H-CMP-1 and H-CMP-G towards thiol-yne reaction, we carried out the density functional theory (DFT) calculations within periodic boundary conditions. For the

geometrical optimization calculations, the Perdew-Burke-Ernzerhof (PBE)/light-tier-1 level of theory with a 1×1×1 mesh of *k*-points was used, and the convergence criteria was set to 0.01 eV/Å. We designed the ideal network structures of H-CMP-1 and H-CMP-G having a planar and hexagonal shape, as shown in Fig. S7. Herein, it should be noted that actual systems would have an amorphous structure. To eliminate interaction between slabs along the z-axis, the vacuum space of 30 Å was added and the lattice parameter *c* was fixed. Both atomic positions and lattice parameters only except *c* were fully optimized for H-CMP-1 and H-CMP-G. Then, the model systems (Cases 1–4 in Fig. S7) were designed to estimate the strain energies that arise from thiol addition to these ideal network structures according to alkyne carbon sites. In order to reduce the computational costs, the propyl group in 1-propanthiol was substituted by a methyl group. To calculate the strain energies, we assumed two conditions as below. We simplified a thiol-yne reaction as the concerted reaction. Rigorously, the radical mediated thiol-yne reaction might consist of a propagation step and a chain transfer step.[5] However, we noted that our proposed reaction scheme would be enough to describe the reaction energy and strain energy for overall (net) reaction instead of the transition state energy for each of the reaction steps.

As the structural strain energies, we considered the changes of self-consistent field (SCF) energies between the optimized structures with and without the constraint options for the fixed positions of benzene rings denoted in Fig. S7. The network structure connected with the benzene rings and alkyne moieties in H-CMP-1 and H-CMP-G might be closely packed by surrounding polymer network structures and disordered in amorphous manner. Thus, the geometrical changes induced by a thiol addition would become the inevitable strains required to complete the reaction. Especially, the benzene rings, bulkier building blocks than alkyne moieties, could receive more constrains than alkyne moieties. Hence, we thought that the difference of SCF energies between the optimized structure having the fixed benzene ring positions and fully relaxed structure could represent most of the structural strain energies accompanying with the thiol addition.

The initial geometry for Cases 1–4 were designed to keep the planarity of H-CMP-1 or H-CMP-G locating a methyl thiyl group ($-SCH_3$) and a hydrogen atom (−H) near an alkyne. First, geometrical optimizations with the fixed benzene ring positions were carried out. Then, based on these optimized geometries, fully relaxed structures were obtained without any atomic constraints. Finally, we defined the strain energy (ΔE_{strain}) as follows: $\Delta E_{strain} = E_{fix} - E_{full}$, where E_{fix} and E_{full} are the SCF energy for optimized structure with the fixed benzene ring positions and the SCF energy for the fully optimized structures, respectively.

For Cases 1–4 calculations, the lattice parameters, that is, α, β, γ and *c* were fixed to avoid the interference between a unit cell and itself. From our tests, severe lattice parameter changes were observed without these lattice parameter constraints, resulting in serious convergence problems as well as interaction between slabs. We thought that this kind of deformation of a unit cell might happen to cancel the net dipole moment of a unit cell. Thus, the length parameters *a* and *b* were fully relaxed to consider the strains for a unit cell changes that result from thiol addition. All DFT calculations were conducted using FHI-aims code.[6]

Reference

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Fig. S1 SEM images of H-CMP-1, H-CMP-Br, H-CMP-G, H-CMP-1-PT, H-CMP-Br-PT, and H-CMP-G-PT.

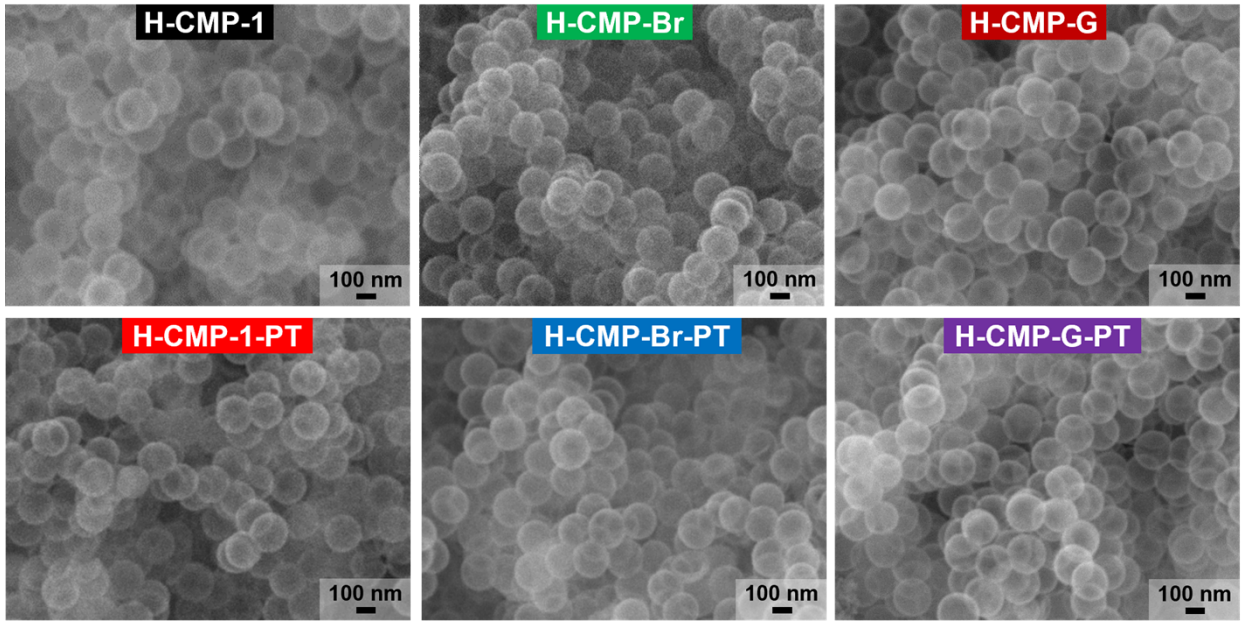


Fig. S2 Additional TEM images of H-CMP-1, H-CMP-Br, H-CMP-G, H-CMP-1-PT, H-CMP-Br-PT, and H-CMP-G-PT.

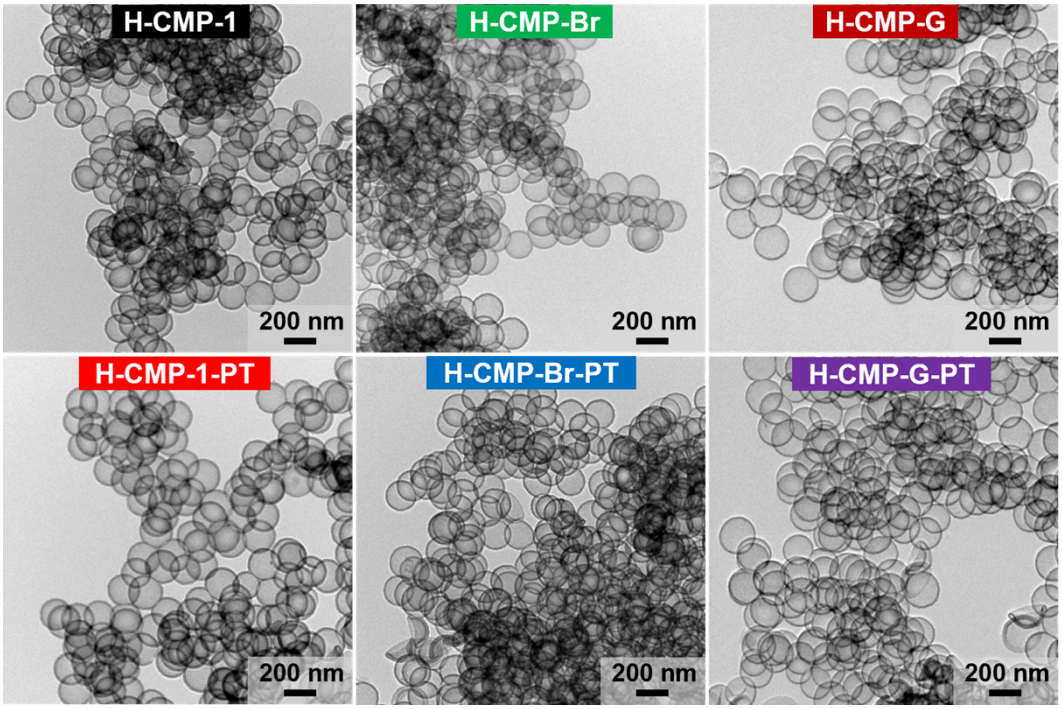


Fig. S3 N_2 adsorption-desorption isotherm curves obtained at 77K and pore size distribution diagrams of H-CMP-1, H-CMP-Br, H-CMP-G, H-CMP-1-PT, H-CMP-Br-PT, and H-CMP-G-PT.

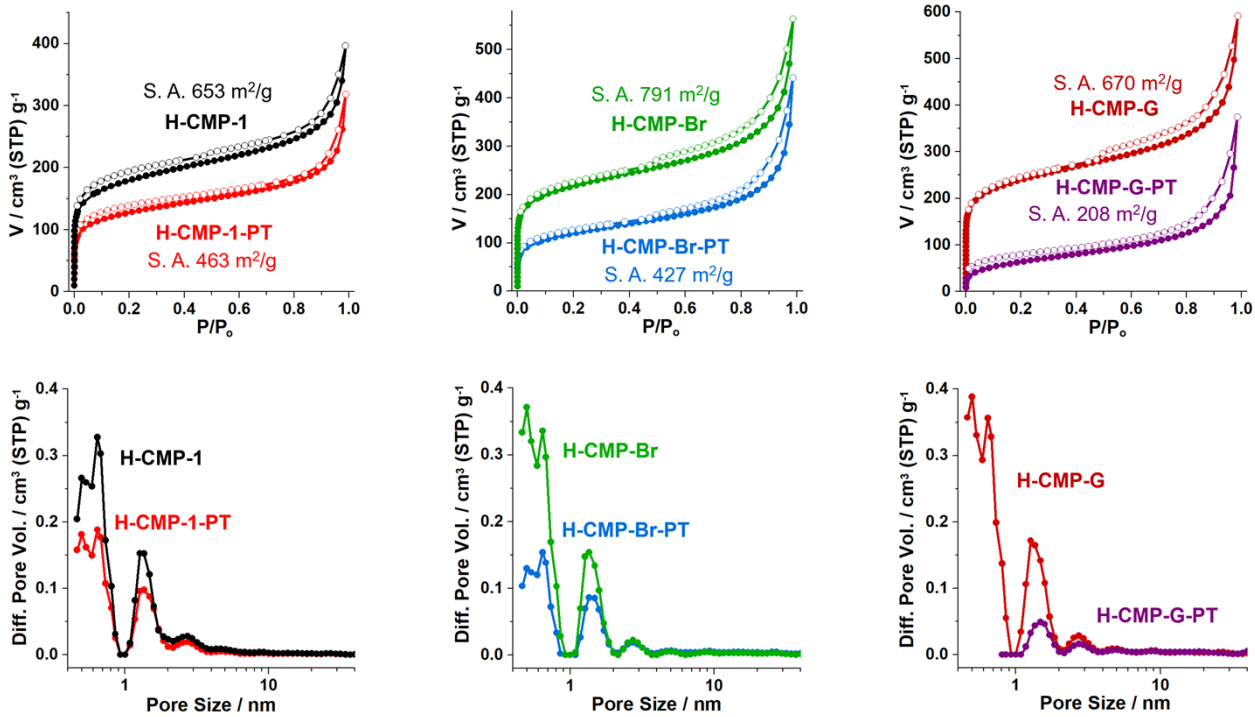


Fig. S4 IR absorption spectra of H-CMP-1, H-CMP-Br, H-CMP-G, H-CMP-1-PT, H-CMP-Br-PT, and H-CMP-G-PT.

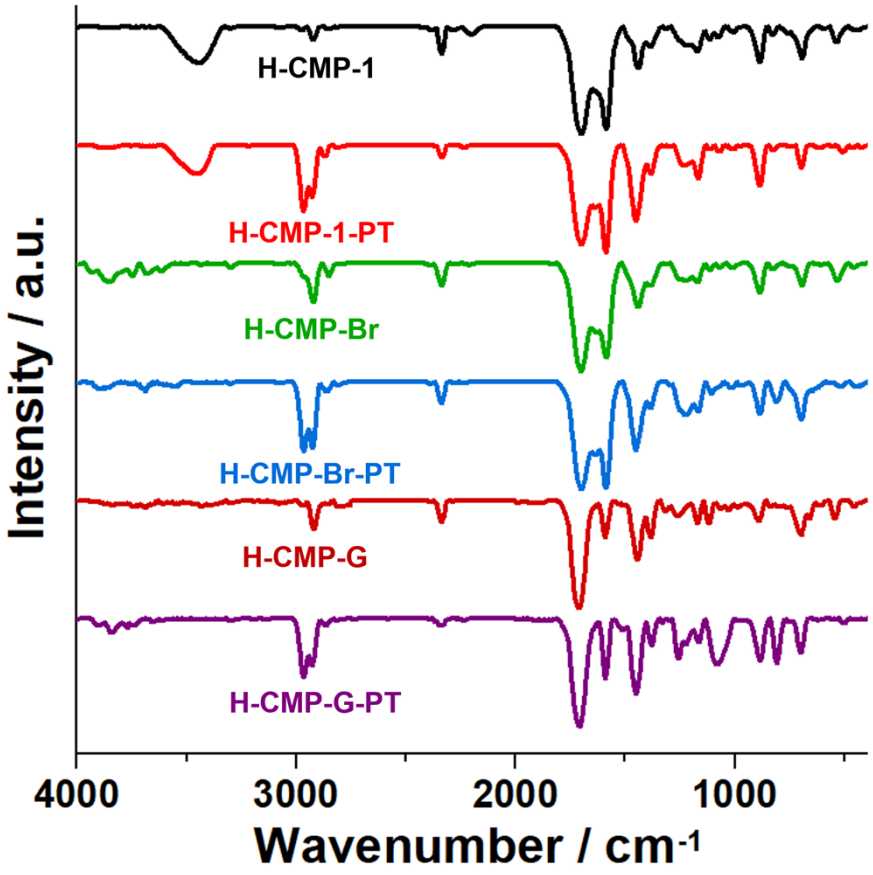
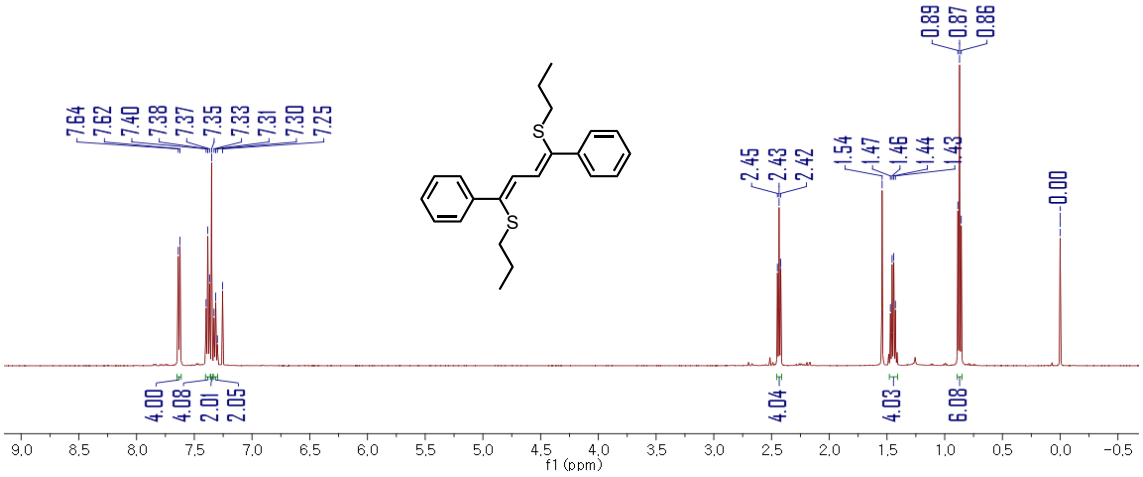


Fig. S5 ^{1}H and ^{13}C NMR spectra of a double 1-propanethiol adduct (an unknown compound) to 1,4-diphenyl-1,3-butadiyne.



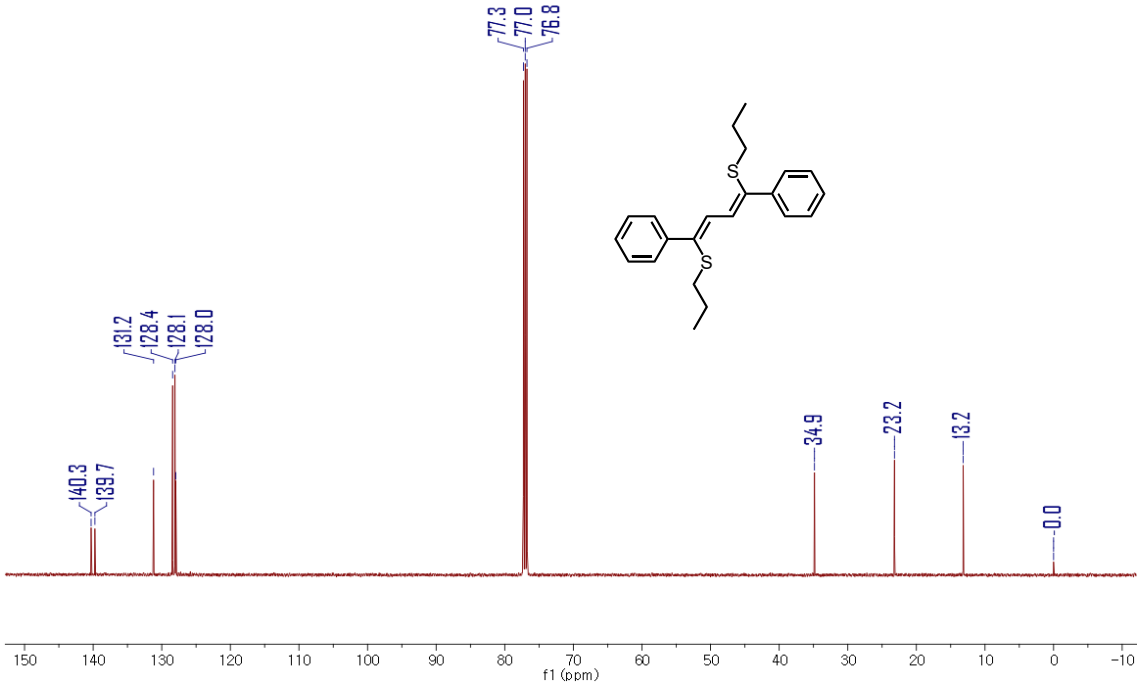


Fig. S6 ^{13}C NMR spectra of diphenylacetylene, 1,4-diphenyl-1,3-butadiyne, and their 1-propanethiol adducts.

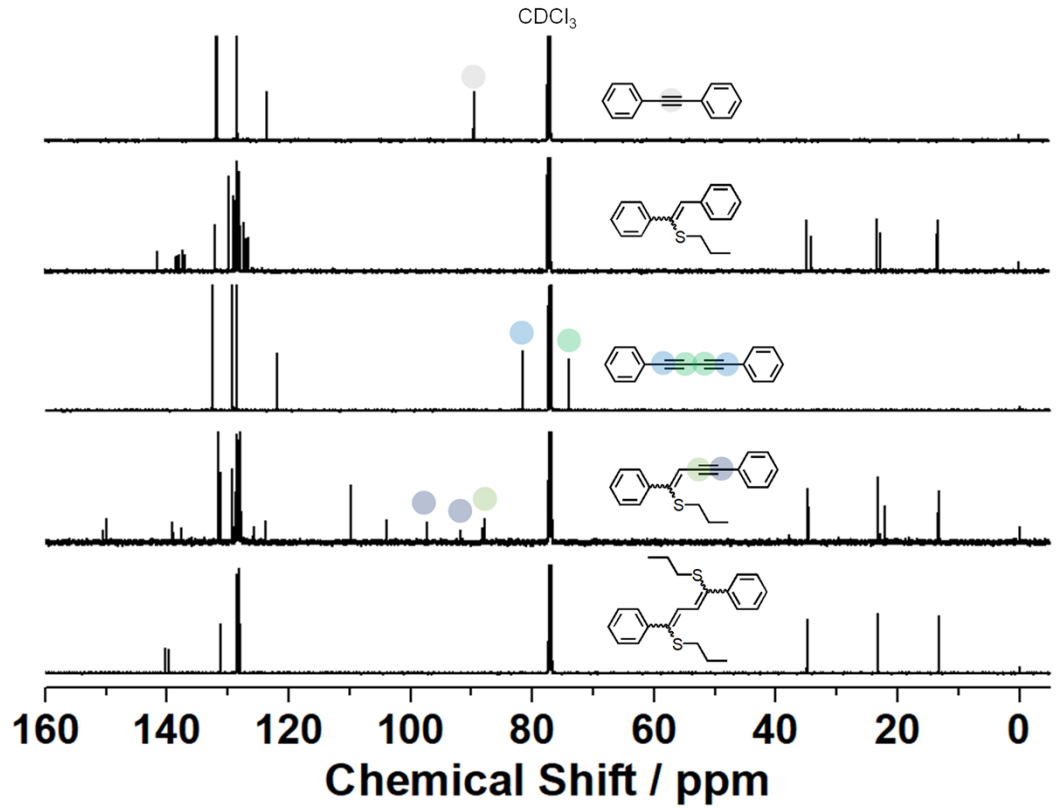


Fig. S7. The designed model systems for ideal network structures of H-CMP-1 and H-CMP-G to calculate structural strain energies of the thiol addition reaction, and their optimized structures with/without constraints of benzene positions using DFT method.

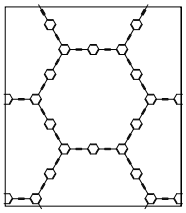
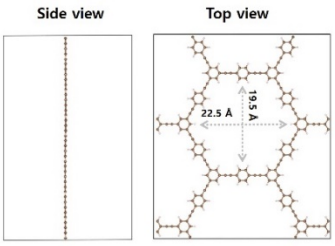
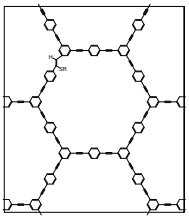
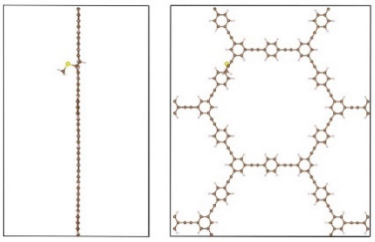
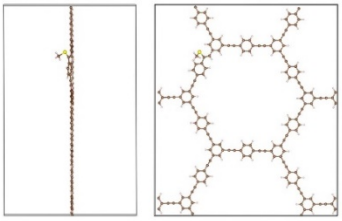
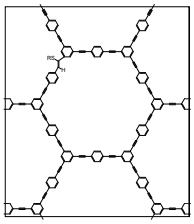
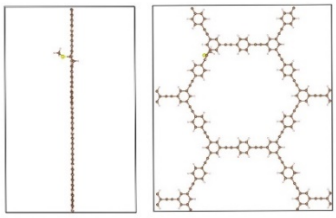
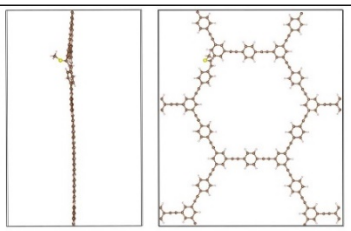
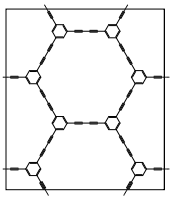
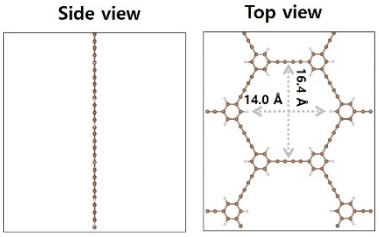
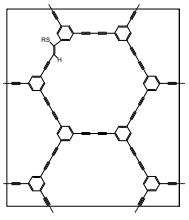
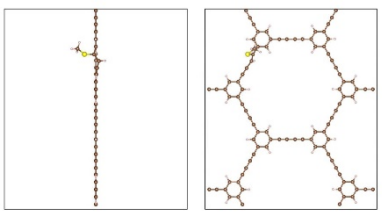
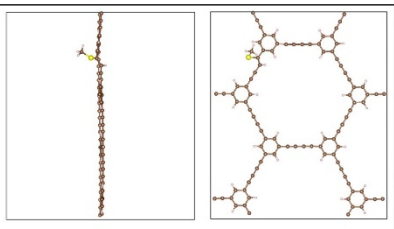
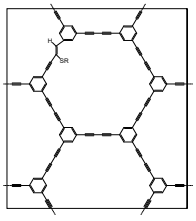
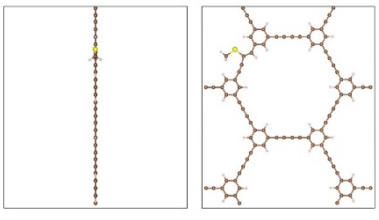
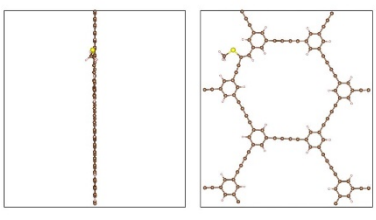
Model	Schematic figures	Optimized structures		Strain Energy (ΔE_{strain} in Kcal/mol)
		Optimization with the fixed benzene rings	Full optimization without the fixed benzene rings	
H-CMP-1				
Case 1				11.12
Case 2				11.60
H-CMP-G				
Case 3				6.38
Case 4				4.33

Fig. S8 The calculated self-consistent field (SCF) energies (in eV) and strain energies (in kcal/mol) in the main chain post-synthetic modification by thiol-yne reactions based on the model systems. The strain energy is defined as $\Delta E_{strain} = E_{fix} - E_{full}$, where E_{fix} and E_{full} are the SCF energy for optimized structure with the fixed benzene ring positions and the SCF energy for fully optimized structures, respectively.

Model systems	**$HSCH_3$**	**H-CMP-1**	**Case 1**	**Case 2**	**H-CMP-G**	**Case 3**	**Case 4**
SCF energy for fully optimized structures (E_{full} in eV)	-11932.46075306	-175194.61568583	-187128.40228361	-187128.41248395	-99816.55291279	-111750.34566598	-111750.32288047
SCF energy for optimized structures with fixed benzene rings (E_{fix} in eV)			-187127.91989434	-187127.90967828		-111750.06896514	-111750.13514689
Strain Energy (ΔE_{strain} in kcal/mol)			11.12	11.60		6.38	4.33

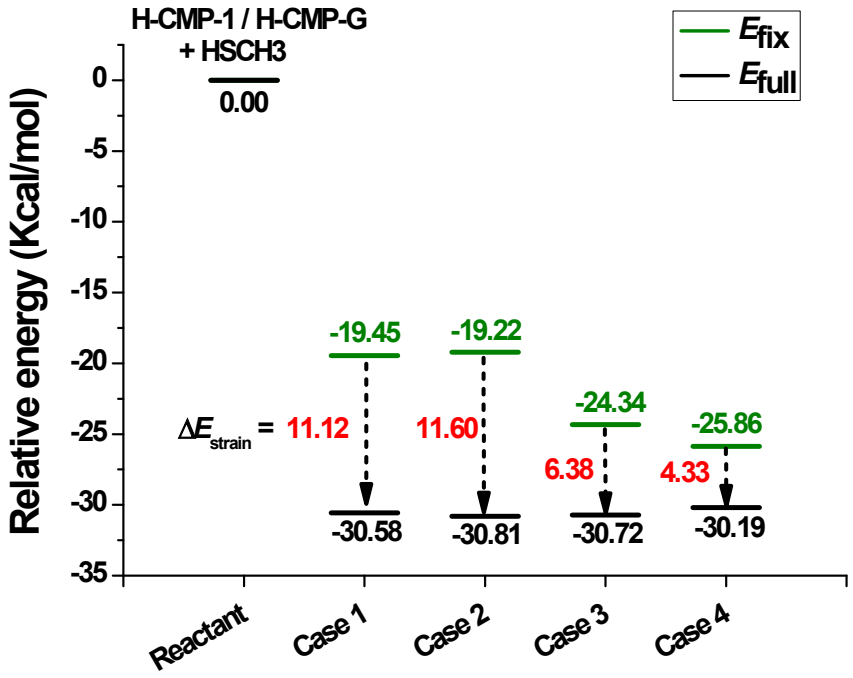


Fig. S9 The cartesian coordinates (in Å) of optimized geometries for the ideal structures of H-CMP-1 and H-CMP-G and for the structures of Case 1–4.

H-CMP-1

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Case 1_full

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Case 3_full

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Case 4_full

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C 3.313949347 19.588510513 14.927808762
C 4.124318123 18.436500549 14.934403419
C 5.530392647 18.553062439 14.934174538
C 6.126057625 19.832252502 14.927251816
C 5.324041843 20.991998672 14.918521881
C 8.156394005 14.039539337 14.955565453
C 7.584144592 15.127392769 14.949933052
C 6.930016518 16.308773041 14.943906784
C 6.316773415 17.374156952 14.938596725
C 8.802713394 28.879314423 15.023215294
C 8.058595657 27.679647446 15.018531799
C 8.698472977 26.421020508 15.013595581
C 10.112138748 26.402236938 15.027392387
C 10.870480537 27.588424683 15.028655052
C 10.209511757 28.834491730 15.024024963
C 18.232398987 28.680498123 15.034925461
C 17.510520935 27.468765259 15.032025337
C 18.209535599 26.243942261 15.027547836
C 19.618959427 26.226213455 15.026071548
C 20.330656052 27.442724228 15.029329300
C 19.642160416 28.672498703 15.033829689
C 12.286382675 27.538610458 15.032546043
C 13.515294075 27.514812469 15.035952568
C 14.865292549 27.494541168 15.035369873
C 16.094326019 27.481712341 15.033978462
C 20.324440002 24.998823166 15.021598816
C 20.959892273 23.947254181 15.016232491
C 21.660074234 22.793762207 15.009321213
C 22.301984787 21.746131897 15.002366066
C 20.315448761 8.710505486 15.025299072
C 26.576007843 19.349637985 14.958971024
C 27.804450989 19.378553391 14.949591637
C 7.968865395 9.132324219 14.980079651
C 7.359137535 8.065093994 14.986918449
C 1.901936293 19.482770920 14.931278229
C 0.674381495 19.426548004 14.940793037
C 8.127655983 30.125650406 15.028624535
C 7.527386665 31.198371887 15.032012939
C 20.370508194 29.886743546 15.038015366
C 21.023290634 30.927782059 15.040642738
C 23.059621811 4.267238617 15.045414925
C 22.379226685 3.033112764 15.046012878

C 23.097690582 1.820295930 15.045570374
C 24.507268906 1.846896410 15.044558525
C 25.197921753 3.076602936 15.044936180
C 24.469152451 4.283993721 15.045615196
C 20.959751129 7.664304733 15.030396461
C 21.670995712 6.517548561 15.035566330
C 22.325309753 5.477606297 15.040156364
C 6.699915886 6.886706352 14.999260902
C 6.112688541 5.806996822 15.010462761
C 4.103162766 2.078593969 15.037429810
C 6.176219940 3.356940031 15.025518417
C 5.440130711 4.560075760 15.021999359
C 4.030896664 4.514002323 15.026575089
C 3.357571840 3.275153637 15.033981323
C 1.941614389 3.230800629 15.036032677
C 0.713307083 3.186978817 15.037840843
C 26.614255905 3.104138851 15.042071342
C 27.842758179 3.142424583 15.039674759
C 5.513124466 2.112475872 15.033347130
C 6.250372887 0.902813554 15.035732269
C 6.856610298 32.370395660 15.033267975
C 22.394794464 0.591198921 15.044464111
C 21.734640121 32.074691772 15.043410301
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C 6.691585541 24.804267883 14.869561195
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C 3.904274702 24.999168396 14.429543495
H 21.253259659 19.287420273 15.009296417
H 25.019571304 17.166666031 14.969777107
H 24.971935272 21.489662170 14.976066589
H 17.713916779 13.355129242 14.998160362
H 17.644474030 9.032434464 15.016316414
H 21.421791077 11.134521484 15.019918442
H 6.975013256 11.633893013 14.960395813
H 10.628237724 9.323339462 14.985906601
H 10.803795815 13.642045975 14.968377113
H 3.293302774 21.750757217 14.913553238
H 3.664540768 17.449378967 14.940078735
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H 10.635918617 25.445402145 15.031675339
H 10.786262512 29.758144379 15.024724960
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H 17.656423569 25.305820465 15.025325775
H 21.419569016 27.432401657 15.028499603
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H 24.999334335 5.235249043 15.044819832
H 7.264836788 3.389250517 15.021325111
H 3.459086418 5.440824509 15.024032593
H 25.066581726 0.912447989 15.043305397
H 3.586346626 1.120018005 15.044735909
H 8.684310913 24.274263382 15.105546951
H 3.993523121 24.347829819 13.552944183
H 3.677371264 24.415287018 15.328490257
H 3.105293036 25.732288361 14.259948730
S 5.393662453 26.005361557 14.657816887

Case 4_fix

C 22.80500000 20.94900000 15.00000000
C 22.09900000 19.72900000 15.00000000
C 22.79600000 18.50400000 15.00000000
C 24.20500000 18.50300000 15.00000000
C 24.91800000 19.71900000 15.00000000
C 24.21400000 20.93900000 15.00000000
C 18.14000000 12.71000000 15.00000000
C 17.43600000 11.48900000 15.00000000
C 18.14900000 10.27400000 15.00000000
C 19.55800000 10.27500000 15.00000000
C 20.25500000 11.50000000 15.00000000
C 19.54900000 12.72000000 15.00000000
C 22.09054766 17.27812333 14.99999978
C 21.49436618 16.20444131 14.99999969
C 20.84003936 15.02551219 14.99999978
C 20.24649866 13.95036731 14.99999986
C 8.68200000 12.69900000 15.00000000
C 7.98400000 11.47500000 15.00000000
C 8.68900000 10.25400000 15.00000000
C 10.09800000 10.26300000 15.00000000
C 10.80300000 11.48300000 15.00000000
C 10.09100000 12.69900000 15.00000000
C 16.02174211 11.48522560 15.00000010
C 14.79365002 11.48550650 15.00000019
C 13.44535453 11.48558569 15.00000022
C 12.21726183 11.48598689 15.00000012
C 4.01500000 20.91800000 15.00000000
C 3.30500000 19.70100000 15.00000000
C 4.01100000 18.48200000 15.00000000
C 5.42000000 18.47500000 15.00000000
C 6.12300000 19.69700000 15.00000000
C 5.42400000 20.92000000 15.00000000
C 7.97648498 13.92506841 15.00000778
C 7.37730291 14.99714809 15.00001355
C 6.71921582 16.17408973 15.00000990
C 6.12162753 17.24706819 15.00000694
C 8.68100000 29.14200000 15.00000000
C 7.98100000 27.91900000 15.00000000
C 8.68400000 26.69700000 15.00000000
C 10.09300000 26.70400000 15.00000000
C 10.80000000 27.92300000 15.00000000
C 10.09000000 29.13900000 15.00000000
C 18.13700000 29.16700000 15.00000000
C 17.43300000 27.94600000 15.00000000
C 18.14600000 26.73100000 15.00000000
C 19.55500000 26.73200000 15.00000000
C 20.25200000 27.95600000 15.00000000
C 19.54600000 29.17600000 15.00000000
C 12.21449175 27.92786377 15.00000014
C 13.44267156 27.93171733 15.00000025
C 14.79089506 27.93628371 15.00000017
C 16.01899575 27.94069353 15.00000009
C 20.26070649 25.50600754 15.00000017
C 20.85773246 24.43271940 15.00000020
C 21.51296283 23.25415837 15.00000017
C 22.10730412 22.17936669 15.00000014
C 20.26486353 9.04962648 14.99999977
C 26.33213946 19.71348722 14.99999936
C 27.56020703 19.70716187 14.99999950
C 7.99037094 9.02411385 14.99999994
C 7.39655049 7.94901034 14.99999987
C 1.89079161 19.70482572 14.99999978
C 0.66264247 19.71154320 14.99999959
C 7.98070524 30.36871492 15.00000367
C 7.38602030 31.44269945 15.00000370
C 20.24693235 30.40699108 14.99999994
C 20.84691058 31.47944726 14.99999989
C 22.82300000 4.50000000 15.00000000
C 22.11900000 3.27900000 15.00000000
C 22.81700000 2.05500000 15.00000000
C 24.22600000 2.05600000 15.00000000
C 24.93800000 3.27200000 15.00000000
C 24.23200000 4.49200000 15.00000000
C 20.86530890 7.97820103 14.99999968
C 21.52437817 6.80168747 14.99999978
C 22.12263525 5.72904288 14.99999986
C 6.74250428 6.76974038 14.99999979
C 6.14717248 5.69548449 14.99999987
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C 6.14300000 3.24500000 15.00000000
C 5.44400000 4.46800000 15.00000000
C 4.03500000 4.46600000 15.00000000
C 3.32500000 3.25000000 15.00000000
C 1.91066228 3.25404439 15.00000000
C 0.68260758 3.26174447 15.00000000
C 26.35210510 3.26708429 15.00000001
C 27.58017106 3.25905261 15.00000001
C 5.44000000 2.02300000 15.00000000
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C 6.73266348 32.62075411 15.00000395
C 22.11010843 0.82745338 14.99999992
C 21.50813242 32.65636334 14.99999985
C 6.07945014 22.22271982 14.99748077
C 6.51330550 23.38187776 14.99400739
C 6.81874205 24.78929448 14.98589831
C 8.09930085 25.31952101 15.00295386
C 3.96343413 24.81151924 14.93525738
H 21.01003849 19.73306126 15.00000173
H 24.74583743 17.55784801 15.00000441
H 24.76143290 21.88038021 15.00002137
H 17.59192892 13.65099593 15.00000035
H 17.60845681 9.32864472 15.00000035
H 21.34396529 11.50394339 15.00000088
H 6.89503130 11.47180002 15.00000236
H 10.64511893 9.32143926 15.00000066
H 10.63248946 13.64378794 15.00000169
H 3.46681771 21.85768125 15.00022809
H 3.46506126 17.53979231 14.99996527
H 7.21207779 19.69382722 14.99969050
H 6.89393312 27.93806090 15.00185053
H 10.64721099 25.76615120 15.00049075
H 10.63330331 30.08287315 14.99991789
H 17.58906656 30.10805420 14.99999971
H 17.60517385 25.78583313 14.99999878
H 21.34094801 27.96015670 15.00000670
H 21.03001071 3.28166400 15.00000089
H 24.77872945 5.43379422 15.00000124
H 7.23200189 3.24291058 15.00000187
H 3.49248958 5.41021220 14.99999990
H 24.76791410 1.11142599 15.00000556
H 3.48496948 1.08879808 15.00000843
H 8.87264099 24.54727494 15.02104392
H 3.94673291 24.17695639 14.04202242
H 3.90936891 24.20785907 15.84825368
H 3.11074211 25.50224500 14.90584571
S 5.41408824 25.89286865 14.94720696

Fig. S10 XRD patterns of H-CMP-1, H-CMP-Br, H-CMP-G, H-CMP-1-PT, H-CMP-Br-PT, and H-CMP-G-PT.