

Supplementary Materials for

**Phase transformation in two-dimensional covalent organic frameworks under
compressive loading**

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1. Supplementary figures

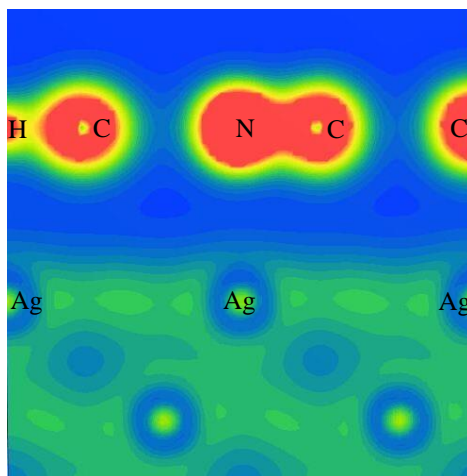


Fig. S1 The electron density of DTPA/Ag(111) interface.

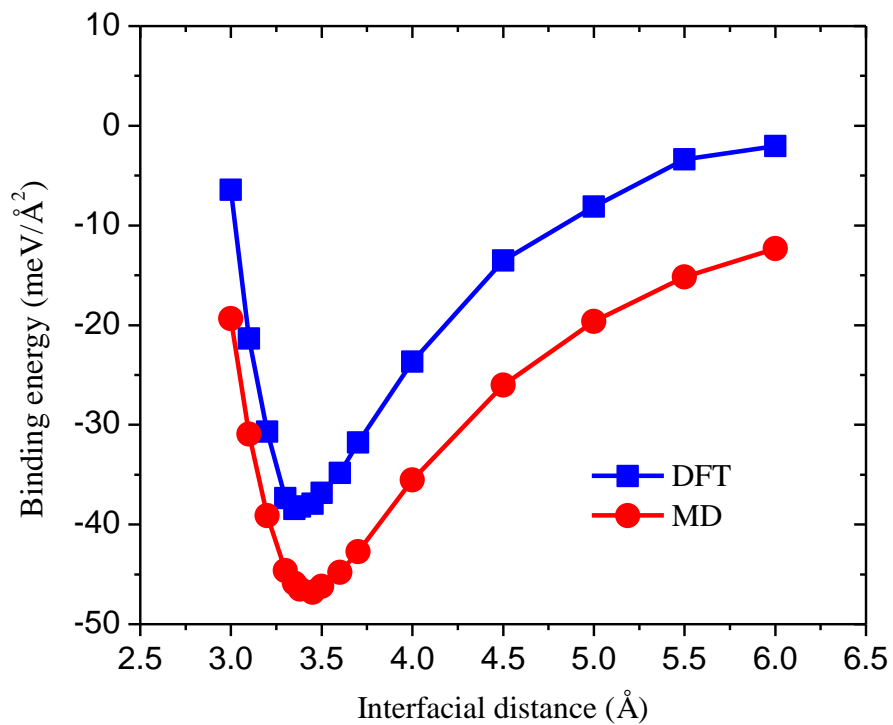


Fig. S2 Relationship between the binding energy of DTPA/Ag(111) interface and the interfacial distance, which was obtained from DFT and MD calculations.

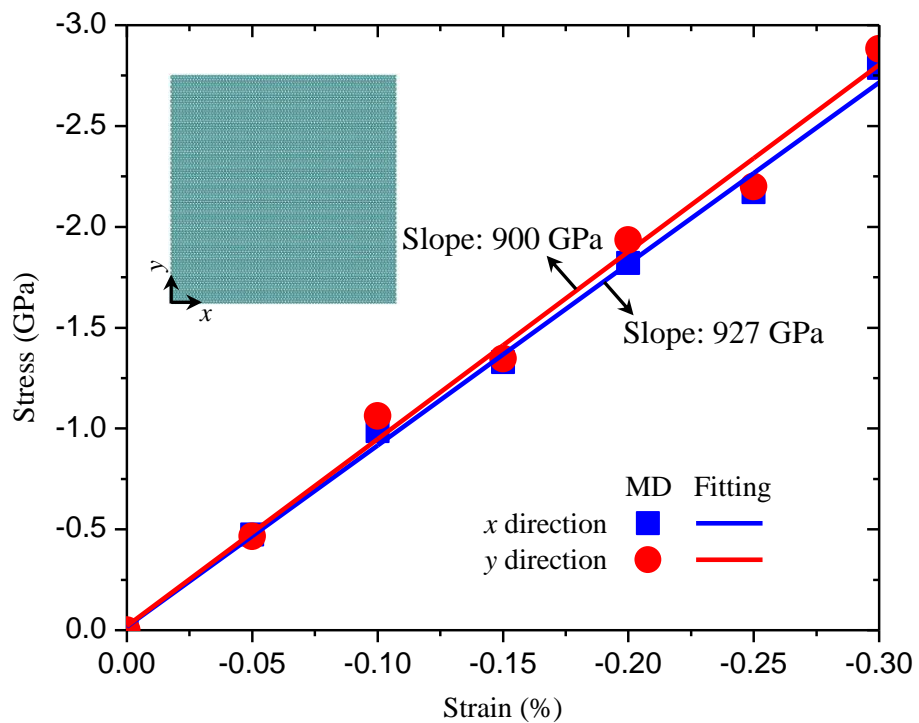


Fig. S3 Stress-strain curves of a 20 nm×20 nm graphene sheet compressed in *x* and *y* directions.

The inset shows the molecular structure of the graphene sheet considered.

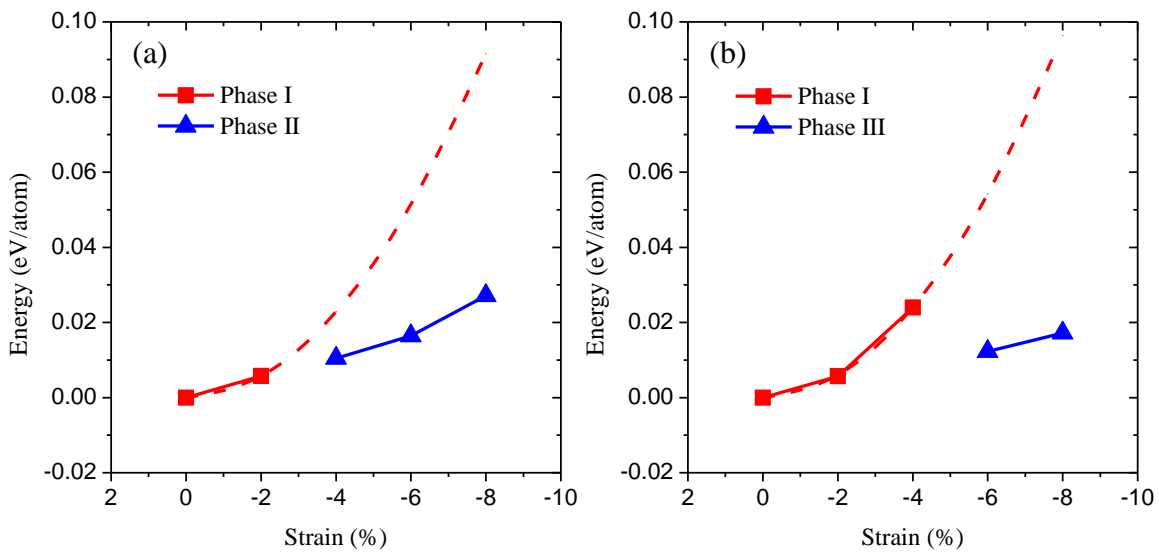


Fig. S4 Relative energy E_R as a function of strain ϵ of DTPA sheets when they are compressed in (a) x direction and (b) y direction. Here the dashed lines are results fitted by $E_R \propto \epsilon^2$.

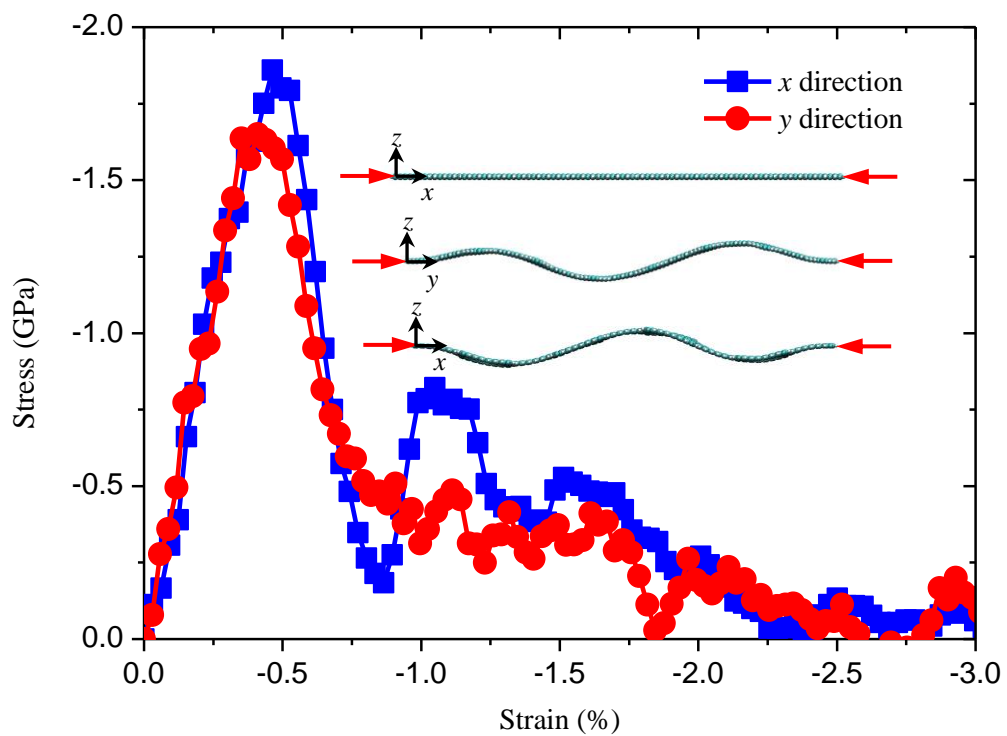


Fig. S5 Stress-strain curves of a freestanding DTPA monolayer subjected to the compression in x and y directions. Here, the insets show the side view of the molecular structure of the DTPA monolayer before and after the buckling instability.

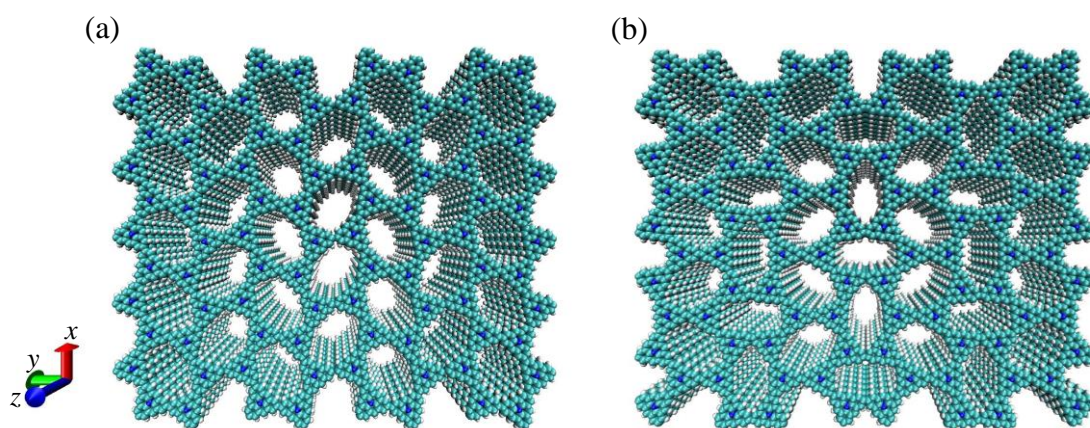


Fig. S6 Crystal structures of the transformed phases of seven-layered DTPA sheets when they are compressed along (a) y direction and (b) x direction.

2. Atomic coordinates of phases I, II and III unit cells of the DTPA sheet

#####Phase I#####

C	74.0650940000	84.6268540000	0.0000000000
C	72.8993912000	85.4179688000	0.0000000000
C	72.8488922000	86.8199463000	0.0000000000
C	75.2296219000	85.4158173000	0.0000000000
C	75.2913895000	86.8197022000	0.0000000000
C	71.6848755000	87.5889435000	0.0000000000
C	74.0698853000	87.5404129000	0.0000000000
C	70.4093781000	89.7296829000	0.0000000000
C	70.3076096000	91.1332016000	0.0000000000
C	71.5961838000	88.9809952000	0.0000000000
C	72.8298569000	89.6764832000	0.0000000000
C	72.8166580000	91.0930405000	0.0000000000
N	74.0665131000	88.9660568000	0.0000000000
C	76.4537201000	87.5887070000	0.0000000000
C	75.3008423000	89.6776810000	0.0000000000
C	75.3143005000	91.0936356000	0.0000000000
C	76.5339966000	88.9806366000	0.0000000000
C	77.7243042000	89.7269287000	0.0000000000
C	77.8251648000	91.1287766000	0.0000000000
C	80.2888947000	91.1976395000	0.0000000000
C	82.7853852000	91.2215424000	0.0000000000
C	85.2779846000	91.1897507000	0.0000000000
C	71.5735245000	91.7453690000	0.0000000000
C	74.0645676000	91.7148896000	0.0000000000
C	76.5610581000	91.7432175000	0.0000000000
C	79.0245285000	91.8151779000	0.0000000000
C	81.5364228000	91.8450624000	0.0000000000
C	79.1261749000	93.2183457000	0.0000000000
C	80.3173752000	93.9648820000	0.0000000000
C	80.4039993000	95.3559723000	0.0000000000
C	81.5492401000	93.2628174000	0.0000000000
C	84.0332947000	91.8449478000	0.0000000000
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C	86.4417420000	93.2071152000	0.0000000000
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H	85.2819311805	90.1012881736	0.0000000000
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H	69.4657930491	89.1860424881	0.0000000000
H	71.5657561754	92.8352832318	0.0000000000
H	74.0532579472	92.8069370879	0.0000000000
H	76.4874728446	92.8259260827	0.0000000000

#####Phase II#####

C	55.3841515000	52.4198380000	0.0000000000
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C	54.1921501000	57.9067422000	0.0000000000
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C	57.8173523000	59.2386398000	0.0000000000
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C	61.5410767000	58.5996971000	0.0000000000
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H	69.3091999761	73.8980497997	0.0000000000
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H	58.7109953202	52.5135377234	0.0000000000
H	54.5890496122	51.6687532603	0.0000000000
H	52.9446506287	53.5149046103	0.0000000000
H	51.2581009770	55.2942620148	0.0000000000

#####Phase III#####

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C	79.4850769000	39.8125687000	0.0000000000
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C	61.1722641000	43.0332184000	0.0000000000
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C	57.1117859000	47.7573815000	0.0000000000
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C	60.6866837000	45.7655487000	0.0000000000
C	61.9842148000	45.3113175000	0.0000000000

C	63.0277863000	46.2039566000	0.0000000000
C	64.3475113000	45.8201981000	0.0000000000
C	66.9229736000	45.0727615000	0.0000000000
C	66.6749726000	46.4624787000	0.0000000000
C	65.3344193000	46.7929268000	0.0000000000
C	68.9518510000	46.8380852000	0.0000000000
C	67.6784973000	47.3838463000	0.0000000000
C	70.1096268000	47.5704308000	0.0000000000
C	71.3106842000	46.9117242000	0.0000000000
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C	73.6688996000	46.8312683000	0.0000000000
C	74.9415054000	47.3761749000	0.0000000000
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C	75.9439164000	46.4511605000	0.0000000000
C	77.2843399000	46.7847748000	0.0000000000
C	78.2728577000	45.8163071000	0.0000000000
C	80.6400070000	45.3135071000	0.0000000000
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C	68.9142762000	51.0200195000	0.0000000000
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N	71.3122940000	49.6837349000	0.0000000000
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C	71.3100662000	51.0970650000	0.0000000000
C	72.5281067000	48.9633142000	0.0000000000
C	72.5414963000	51.8064041000	0.0000000000
C	74.9248810000	48.7843972000	0.0000000000
C	73.7818604000	49.6215363000	0.0000000000
C	73.7053528000	51.0195351000	0.0000000000
C	52.2553558000	56.4745827000	0.0000000000
C	54.5562897000	53.4350472000	0.0000000000
C	53.4132691000	54.2550278000	0.0000000000
C	53.3928070000	55.6603241000	0.0000000000
C	54.6433411000	56.3324242000	0.0000000000
C	55.7475510000	54.1924667000	0.0000000000

C	55.8560486000	55.5943566000	0.0000000000
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C	70.1450882000	56.1752892000	0.0000000000
C	71.3109284000	53.9973602000	0.0000000000
C	71.3099365000	55.3814774000	0.0000000000
C	72.4783860000	53.2068329000	0.0000000000
C	72.4773941000	56.1704216000	0.0000000000
C	51.0927429000	58.7363739000	0.0000000000
C	52.2172928000	57.8746452000	0.0000000000
C	51.1096115000	60.1447144000	0.0000000000
C	52.3923798000	60.6661339000	0.0000000000
C	53.4856797000	58.5034180000	0.0000000000
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C	53.5313111000	59.9022636000	0.0000000000
C	54.7518387000	60.5212937000	0.0000000000
C	55.9216462000	58.4375725000	0.0000000000
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C	63.7510758000	63.5358811000	0.0000000000

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