Supporting Information

Band Gap Engineering of two-dimensional Triphenylene-Graphdiyne and its BN analog: A first-principles calculation

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1. Atomic structure of Tp-BNyne unit-cell in VASP POSCAR

H6B9N9C12

1.00000000000000
13.9688768905323091 -0.0000361897967007 -0.0000023256900294
-6.9844697754505729 12.0974541111990330 0.0000047733704824
-0.0000024600041050 0.0000044090500615 14.7705627766065941
H B N C
6 9 9 12
Direct
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0.5429025884495811 0.9442546136776607 0.5000000080695042
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0.5471774891151187 0.5848307742654246 0.4999999825836667
0.0376573745676710 0.4528294813757177 0.4999992779217856
0.4151730079543553 0.9623432047822397 0.5000000231452524
0.6484792534653986 0.8788197192764877 0.5000004168458486
0.1211787926150578 0.7696562693428043 0.5000000075231326
0.2303413667128479 0.3515224284674903 0.5000000234976690
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0.3323408118509327 0.8739328360121884 0.5000000182007699
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0.4382058183219246 0.7712531595928722 0.5000000188744663
0.2287493535164615 0.6669524147479489 0.5000000077631839
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0.1256438558570971 0.3540857265609633 0.5000000124243023
0.2284391716441046 0.8743575975347306 0.5000000004997659
0.6459154826828647 0.7715593392698895 0.5000001314321545
0.3286222370865292 0.4570778475652225 0.5000000026479035
0.1284539113022087 0.6713768332323604 0.5000000219957687
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0.2284092858951620 0.5617597866305227 0.5000000217941598

0.3333517792294121 0.7715924712689659 0.5000000012817989
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0.0285967773353957 0.2590346442064615 0.4999999868314922
0.2304384731217942 0.9714051343316346 0.4999999919655246
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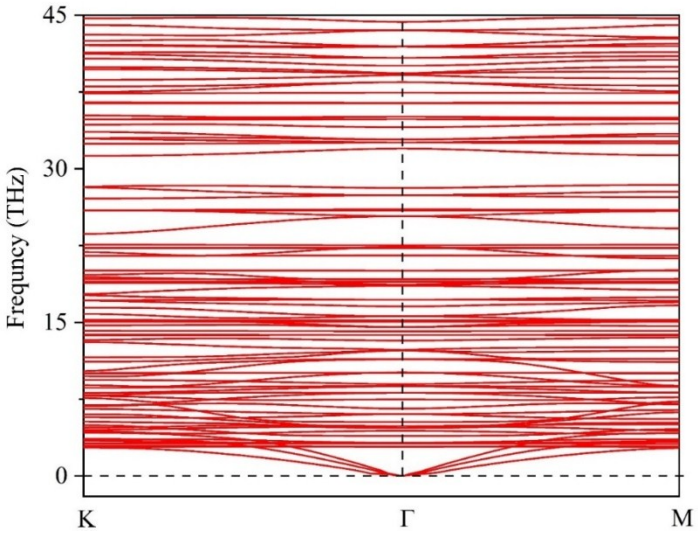
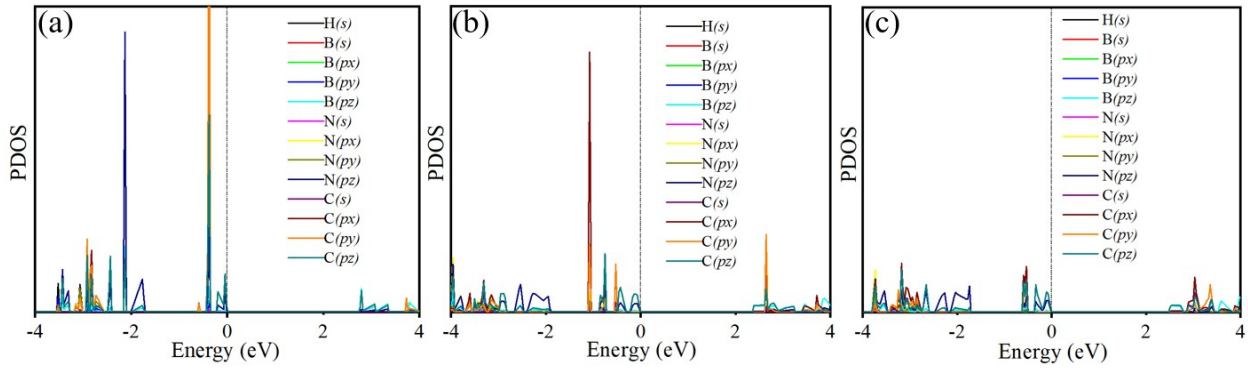


Figure S1 Phonon spectra calculated with 2 × 2 × 1 supercell.



2. PBE results for the PDOS of TpG and its BN-analogous structure.

Figure S2 Partial density of states of Tp-BNyne under (a) 0% (b) 10% Zigzag, and (c) Armchair, uniaxial strain.

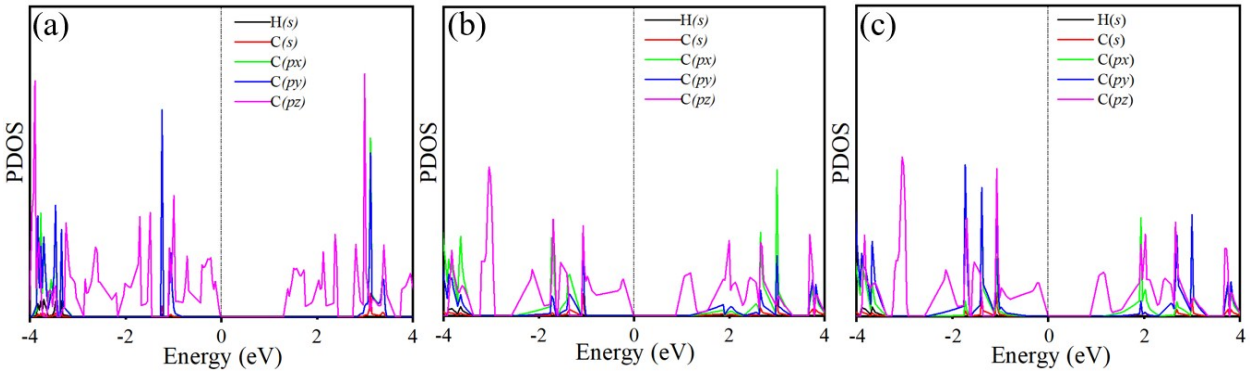


Figure S3 Partial density of states of TpG under (a) 0% (b) 10% Zigzag, and (c) Armchair, uniaxial strain.

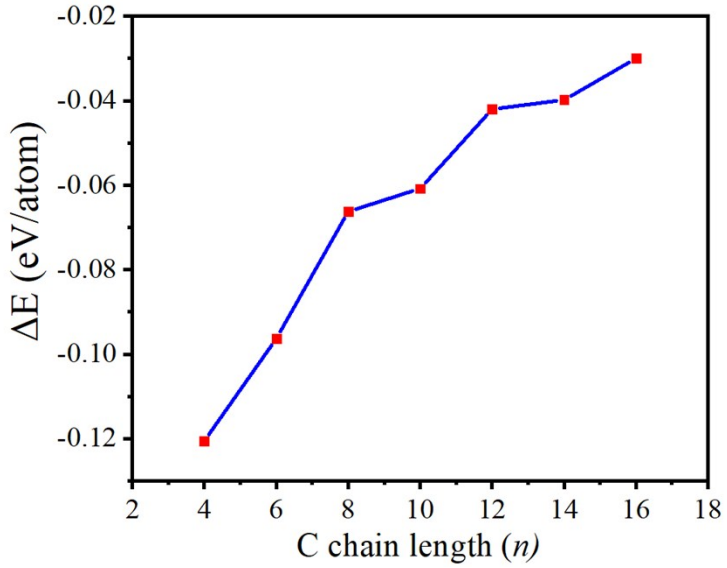


Figure S4 Energetic stability changing with the length of C-chain length *n* in Tp-BNyne.