

Supplementary information

Electronic, Optical, Mechanical and Li-Ion Storage Properties of the Benzotrithiophene-Based Graphdiyne Monolayers Explored by First-Principles and Machine-Learning

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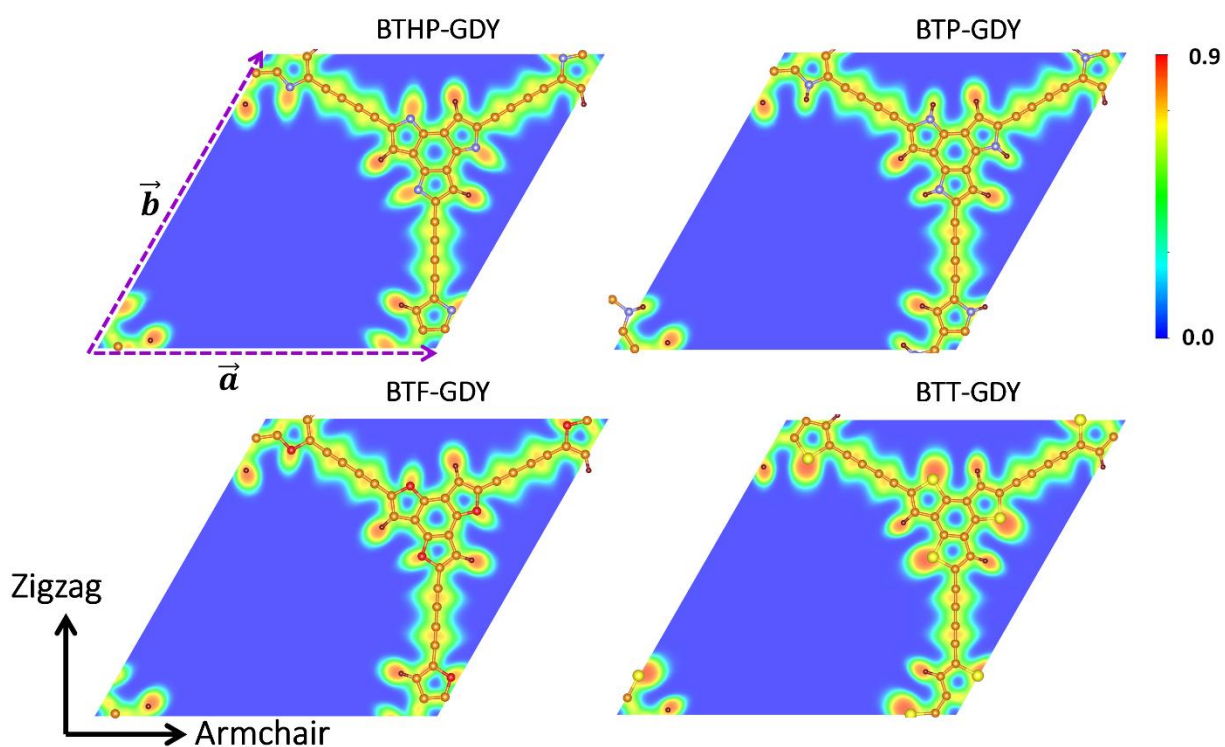


Figure S1, Top views of the molecular structure of benzotrithiophene (BTT: $C_{12}S_3H_6$), benzotripyrrol (BTP: $C_{12}N_3H_9$), benzotrifuran (BTF: $C_{12}O_3H_6$), and benzotri(1H-Pyrrol-1-yl) (BTHP: $C_{12}N_3H_6$) and their corresponding graphdiyne (GDY) lattices (BTHP-GDY, BTP-GDY, BTF-GDY, BTT-GDY). Horizontal and vertical directions are so-called zigzag and armchair, respectively. For each one, contour depicts the electron localization function over the polymer surface with a distance of 0.75 Å. Brown, dark brown, blue, red, and yellow circles represent C, H, N, O, and S atoms, respectively.

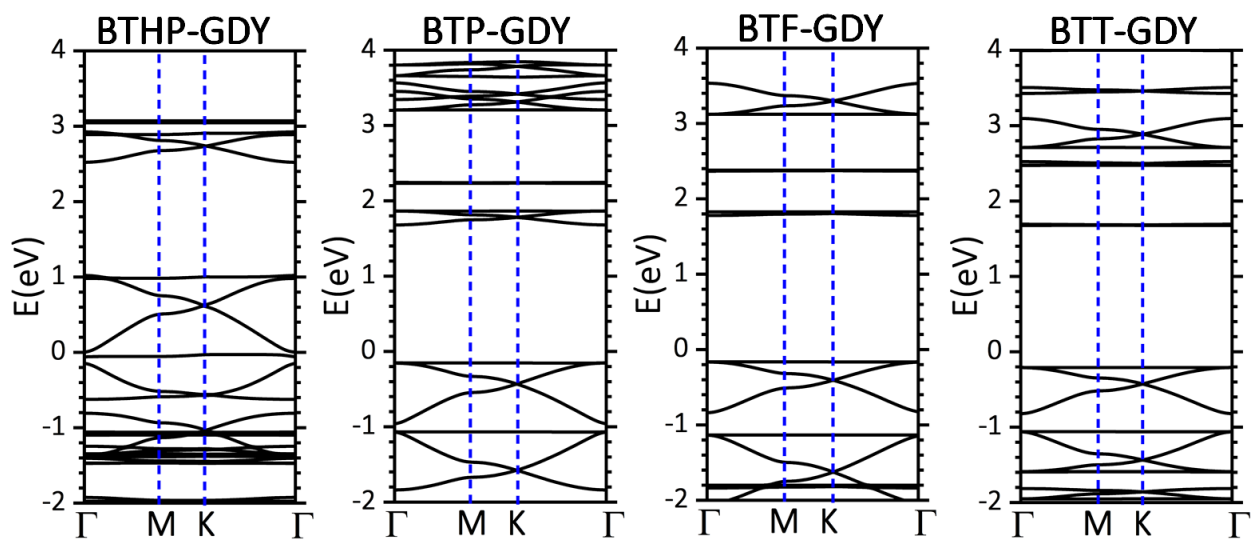


Figure S2, Electronic band structures predicted by PBE method for the BTX-GDY monolayers (Fermi level is set to 0 eV).

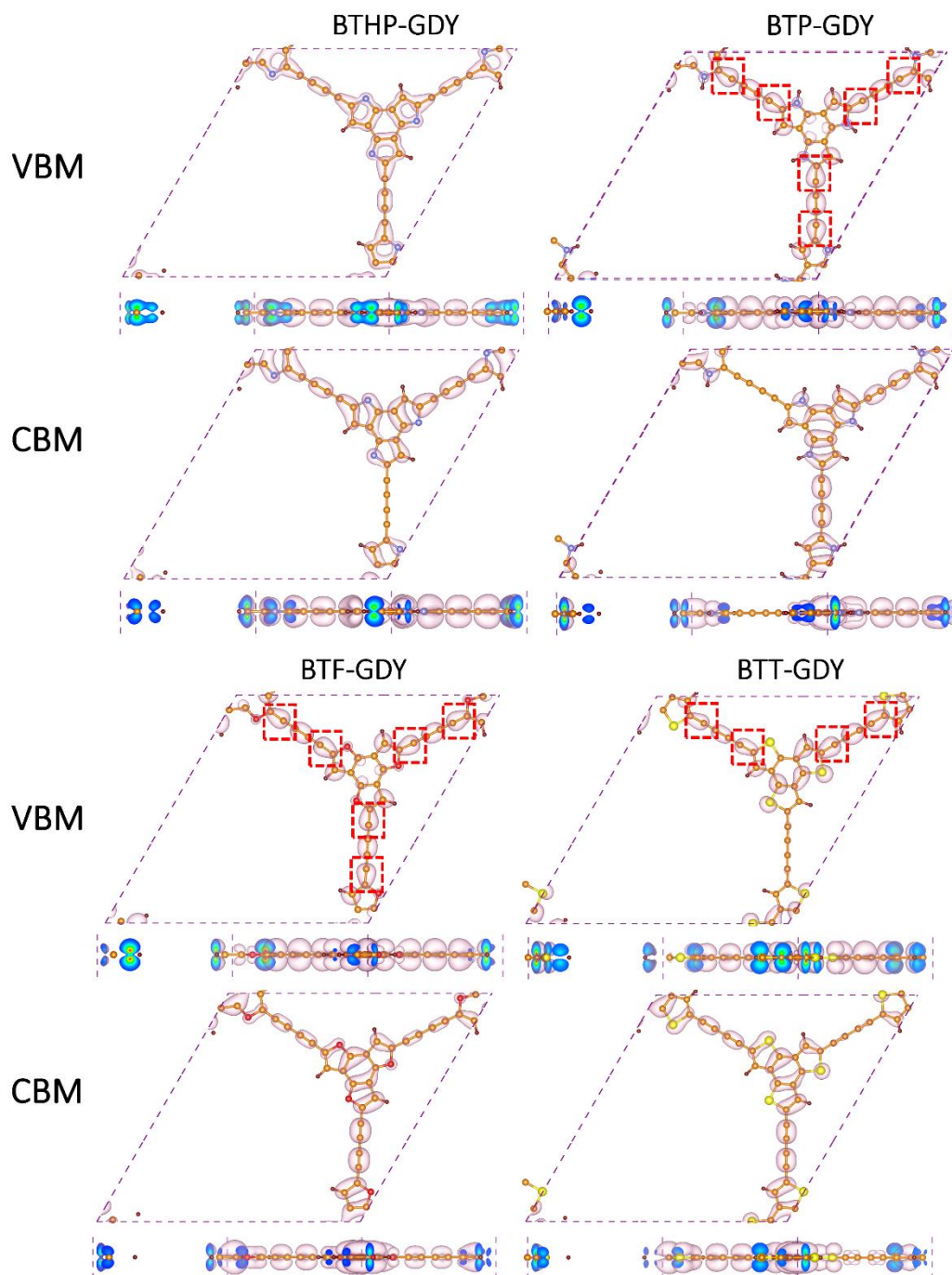


Figure S3, Charge density distributions at VBM and CBM of BTX-GDYs. For all cases, the iso-surface is set to $0.001 \text{ e}/\text{\AA}^3$. Red dashed rectangles indicate bonding interaction between a p-state of BTX molecule and p*-state of diacetylene linkers.

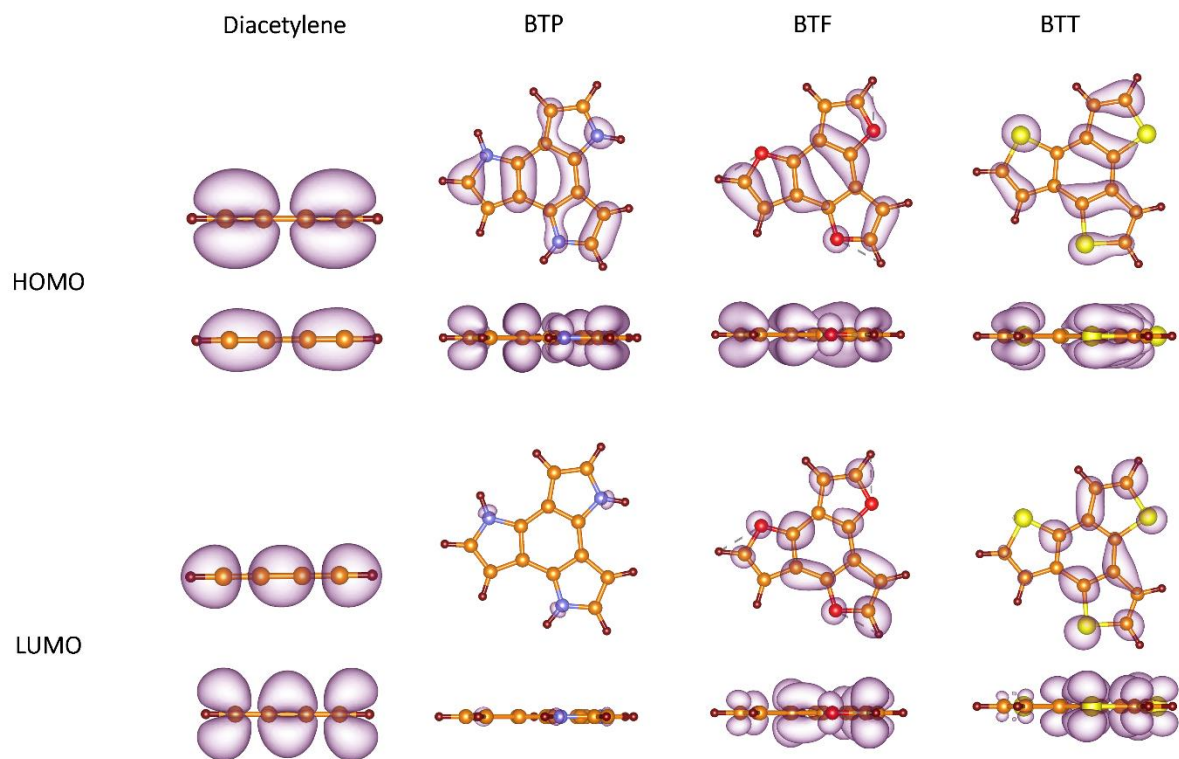


Figure S4, Charge density distributions of HOMO and LUMO states of BTX (X= P, F, T) molecules. For all cases, the iso-surface is set to $0.0025 \text{ e}/\text{\AA}^3$.

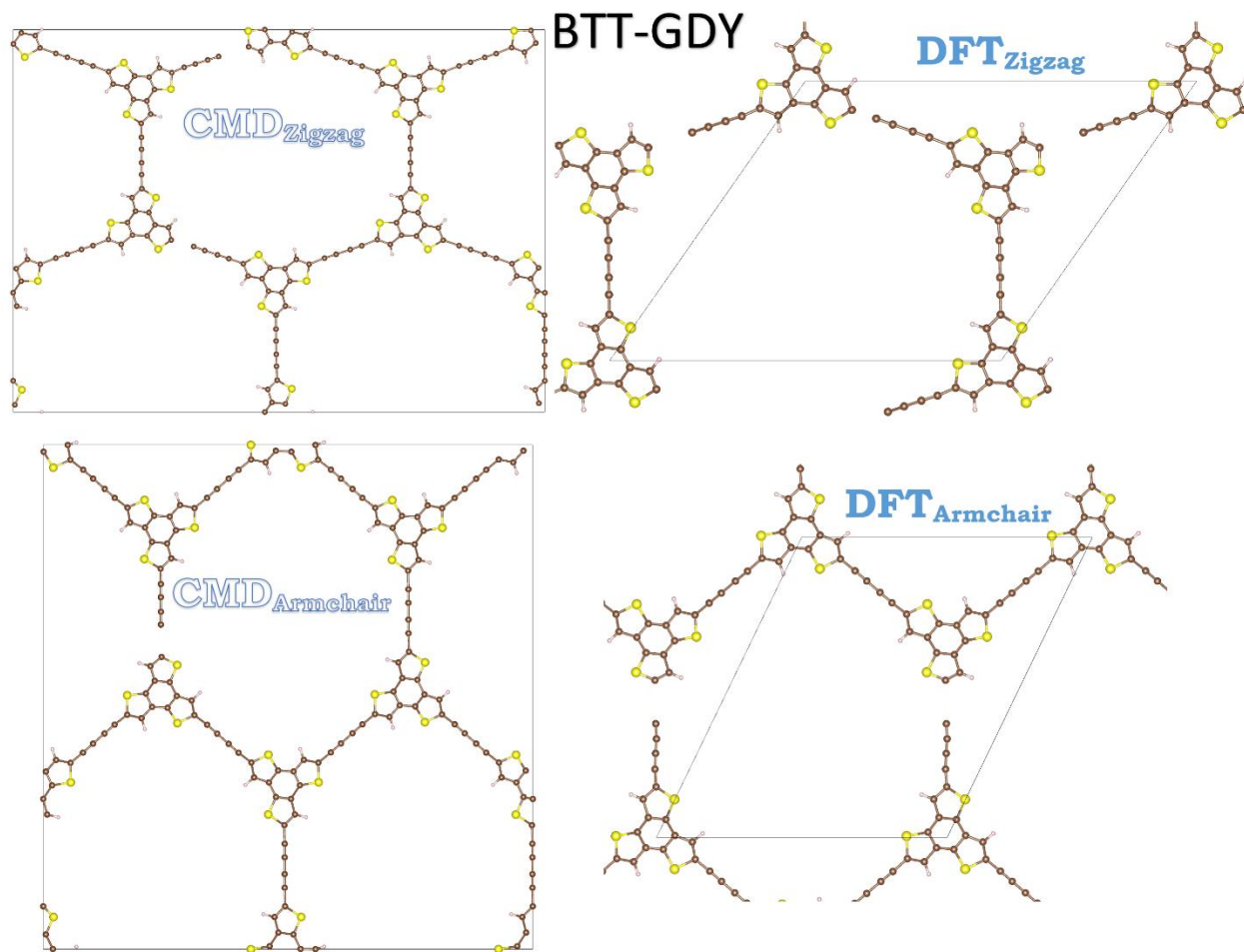


Figure S5, Failure mechanism of the BTT-GDY monolayer predicted by the DFT and MLIP-based CMD method for the uniaxial loading along the zigzag and armchair directions.

Atomic lattices in VASP POSCAR format.

BTT-GDY

```
1.0000000000000000
23.6704400508862243    0.0000000000000000    0.0000000000000000
11.8299906448121757    20.5456758592951196    0.0000000000000000
0.0000000000000000    0.0000000000000000    15.0000000000000000
  C      S      H
 36      6      6
Direct
0.0603711625072217    0.9959019994315569    0.5000000000000000
0.9356688903120689    0.0059260714179520    0.5000000000000000
0.9395668124328201    0.0638925461151121    0.5000000000000000
0.0023575075955263    0.0576594865605726    0.5000000000000000
0.8888673304007421    0.1300010156613207    0.5000000000000000
0.9118447495715241    0.1735686642145018    0.5000000000000000
0.8766686068753875    0.2412712208425490    0.5000000000000000
0.8472835251342693    0.3012198284774969    0.5000000000000000
0.8147412905657685    0.3665676797763405    0.5000000000000000
0.7854543889088913    0.4265020272907140    0.5000000000000000
0.7501762880813522    0.4942056317646251    0.5000000000000000
0.7729991428077964    0.5378789855377016    0.5000000000000000
0.7221840651705570    0.6039246143306362    0.5000000000000000
0.6594154809913219    0.6100777848982030    0.5000000000000000
0.6013645466593086    0.6718395830992466    0.5000000000000000
0.6076433562038401    0.7283087792615192    0.5000000000000000
0.6695185616671134    0.7245788517494880    0.5000000000000000
0.7260207007377241    0.6619253511772965    0.5000000000000000
0.6850041941656314    0.7752908691794331    0.5000000000000000
0.7515226138445581    0.7525305233520768    0.5000000000000000
0.7840075434920634    0.7878790476743163    0.5000000000000000
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0.8468202383035212    0.8506794186443467    0.5000000000000000
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0.9766227000963845    0.8925318527039982    0.5000000000000000
0.9921269762394485    0.9432511292186881    0.5000000000000000
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0.1701900016502399    0.9141024169264333    0.5000000000000000
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0.6644861419785937    0.5349599968825216    0.5000000000000000
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0.8370289451507478    0.1460293009209312    0.5000000000000000
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```

BTP-GDY

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23.1014820338700382	0.0000000000000000	0.0000000000000000
11.5285206518138388	20.0645849672330279	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000

C	N	H
36	6	12

Direct

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0.8792969162939380	0.2386492766676731	0.5000000000000000
0.8483625334840263	0.3000685984582204	0.5000000000000000
0.8145517197189371	0.3670408938826761	0.5000000000000000
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0.7281840376979309	0.6056408859008200	0.5000000000000000
0.6670703239708982	0.6045954737963377	0.5000000000000000
0.6038056398328483	0.6636998977144709	0.5000000000000000
0.6030775915337043	0.7255554162708613	0.5000000000000000
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0.7242528849500053	0.6688238527586647	0.5000000000000000
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BTHP-GDY

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22.8204192407016286	0.0000000000000000	0.0000000000000000
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0.0000000000000000	0.0000000000000000	15.0000000000000000
C	N	H
36	6	6

Direct

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0.9115105951450289	0.1687300192321232	0.5000000000000000
0.8787325265587619	0.2378536917932288	0.5000000000000000
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0.8251963438700958	0.1469462843340235	0.5000000000000000
0.0232407093326635	0.8293701481234801	0.5000000000000000

BTF-GDY

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0.0000000000000000	0.0000000000000000	15.0000000000000000

C	O	H
36	6	6

Direct

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0.8153937960500457	0.3676642717186809	0.5000000000000000
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0.6709894424066931	0.6033431470584460	0.5000000000000000
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