Supporting information for:
Computational Investigation on the Electronic Structure and Functionalities of a Thiophene-Based Covalent Triazine Framework

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Supporting Information

1. Charge density difference plot of AB-stacked bilayer TBCTF.

2. Band structure of bilayer TBCTF in AA stacking mode.

3. Position of VBM and CBM energy levels of difunctionalized and nonfunctionalized g-ZnO/TBCTF composite systems.

4. Noncovalent isosurface plot of hydrogen molecule decorated Li-TBCTF
Figure S1: The (a) Top and (b) side views of charge density difference of AB-stacked bilayer TBCTF. The isovalue of 0.0017 e/Å$^3$ is used. The yellow colour represents charge accumulation, while the blue colour shows charge depletion.
Figure S2: The Band structure of AA-stacked bilayer TBCTF. The Fermi level is indicated by the red dotted line.
Figure S3: The VBM (green) and CBM (red) energy levels of difunctionalized and non-functionalized g-ZnO/TBCTF composite systems (bold) and that of isolated monolayers. The VBM of g-ZnO is set to zero energy.
Figure S4: Gradient isosurfaces for the interaction between the hydrogen molecules and Li-TBCTF. The isosurfaces are coloured on a blue-green-red scale. Blue indicates strong attractive interactions, and red indicates strong nonbonded overlap.