

Figure S1. Side and top representations for the relaxed structures of the vertical and parallel configurations of the $CX_2 \cdots \beta_{12}/GN$ complexes (where $X = O, S, \text{ or } Se$) at all the adsorption sites. Equilibrium distances (d) are given in Å.

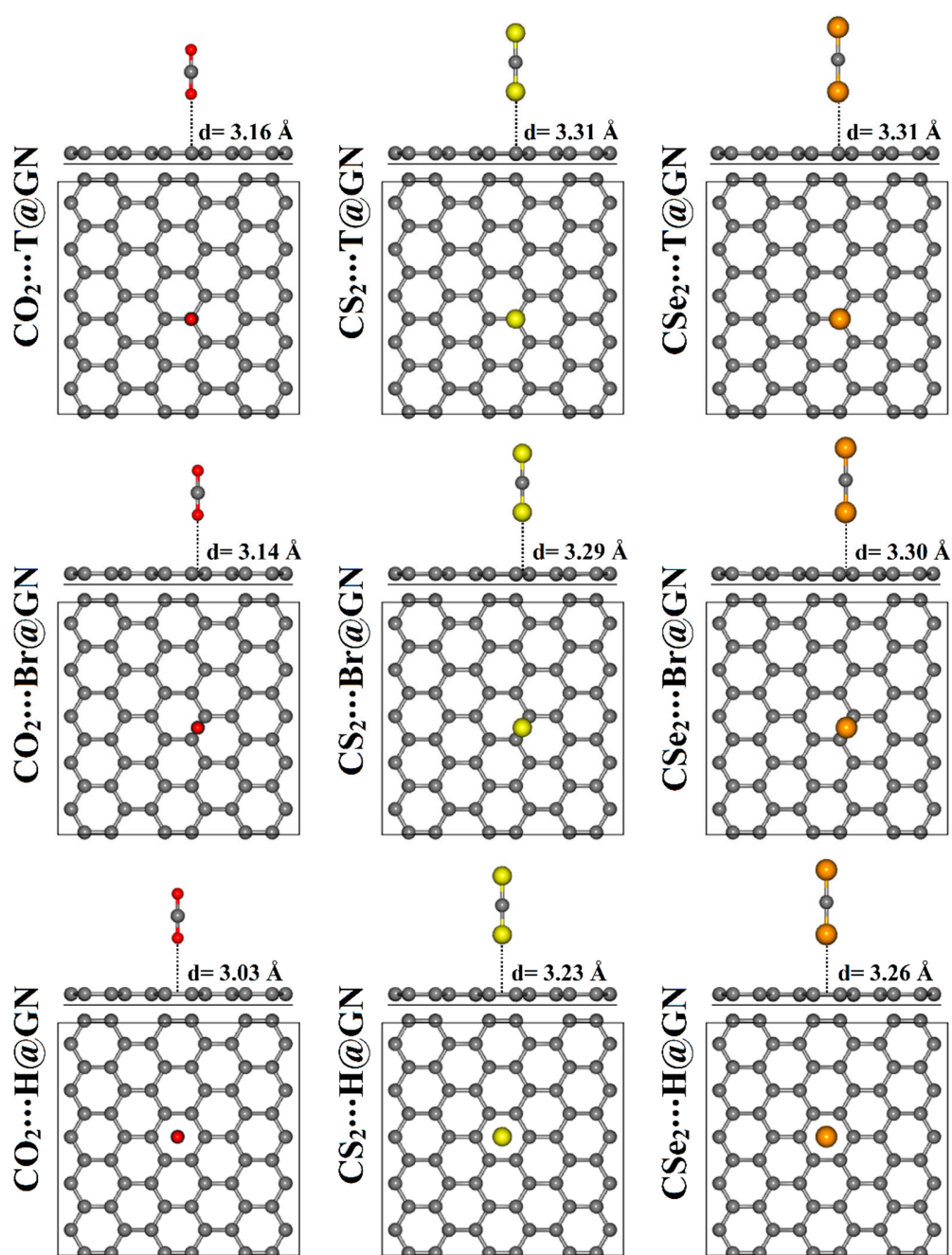


Figure S1. Continued.

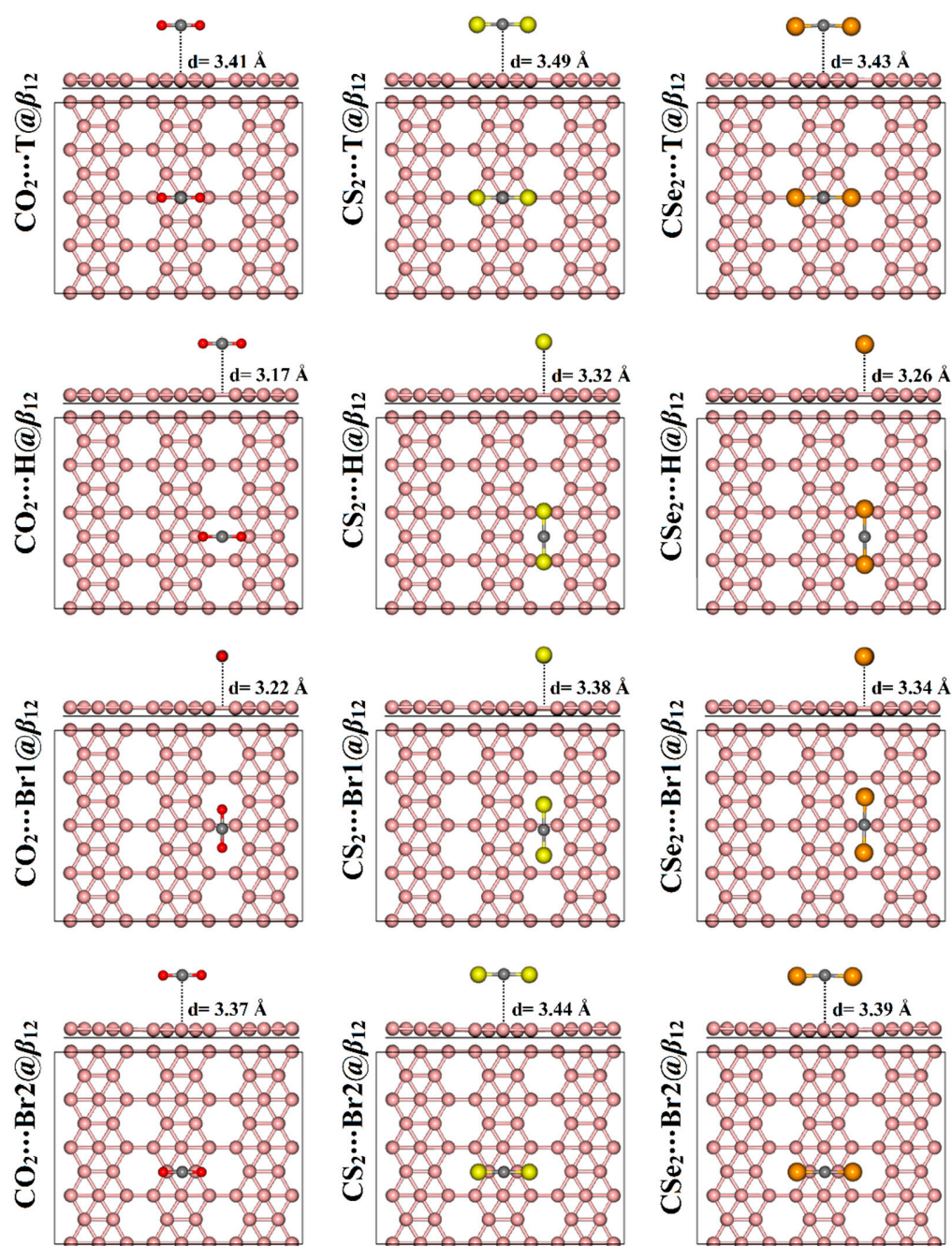


Figure S1. Continued.

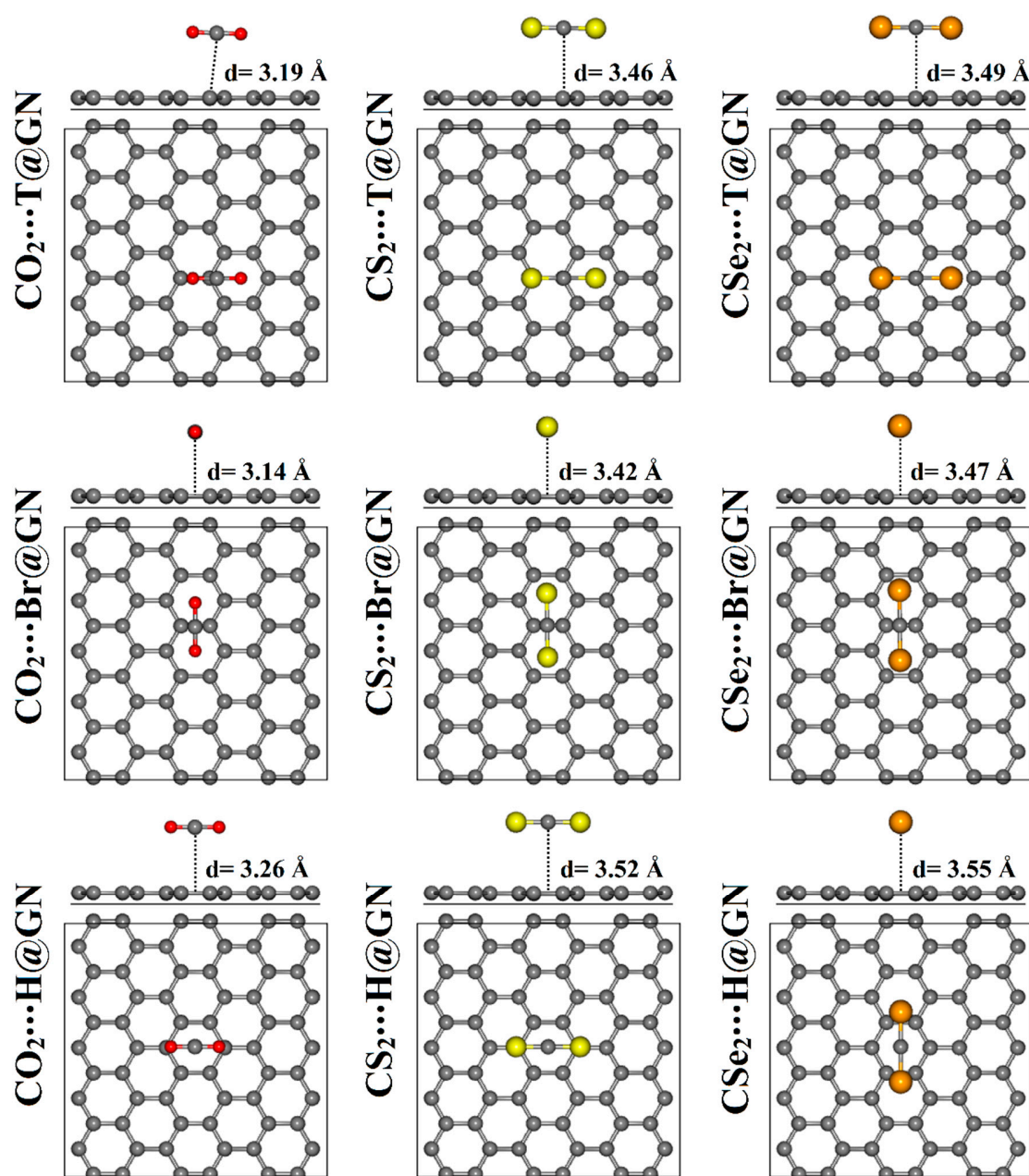


Figure S1. Continued.

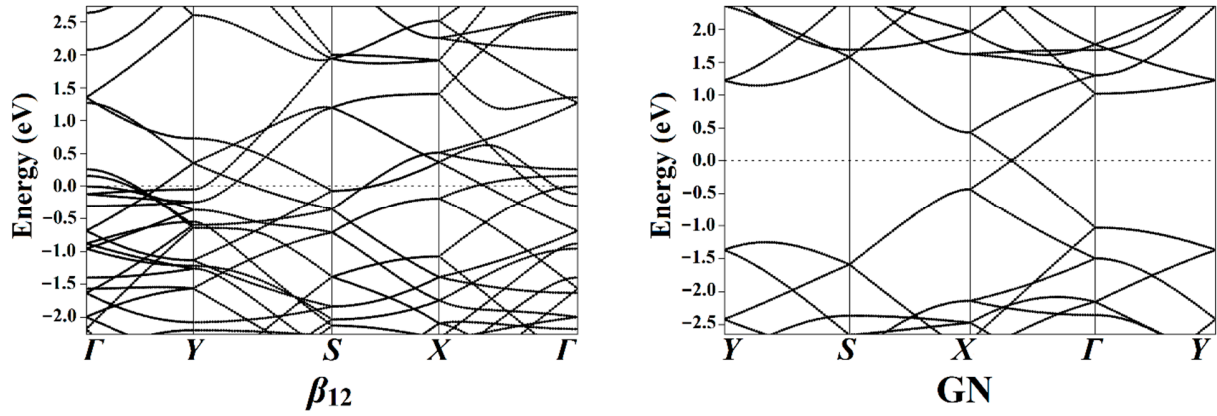


Figure S2. Band structure plots of β_{12} and GN sheets along the high-symmetry points of the Brillouin zone. The Fermi energy is located at zero-energy.

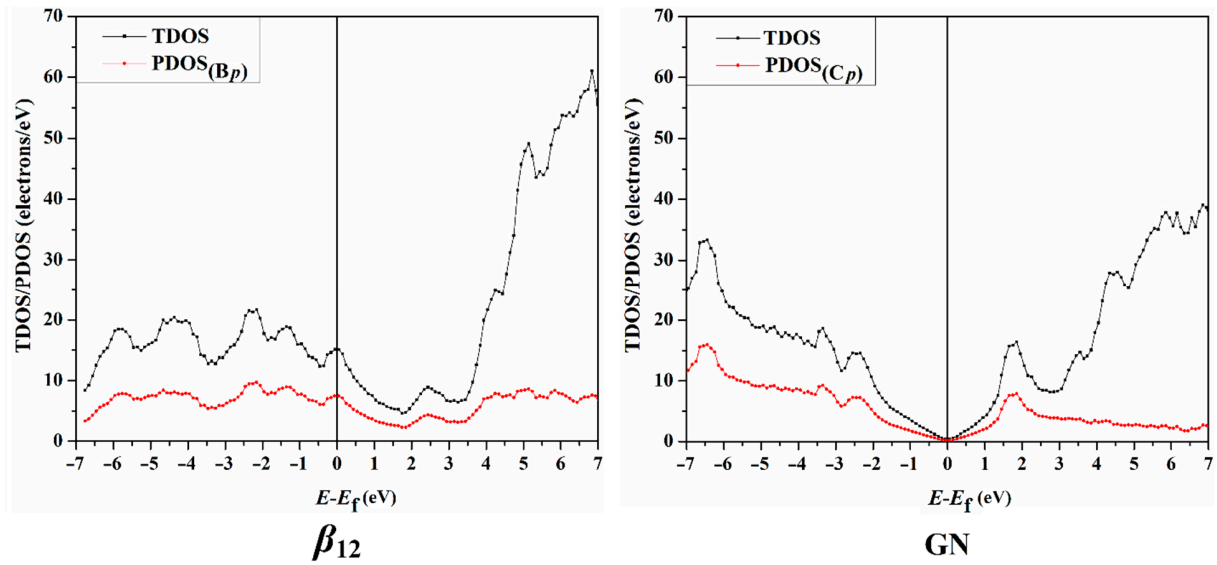


Figure S3. Total and projected densities of states (TDOS/PDOS) plot for the pure surfaces of β_{12} and GN sheets, assuming the Fermi level as the reference level. The contributions of the p -orbital for boron (B) and carbon (C) atoms are represented by B_p and C_p , respectively.

The crystallographic data of the relaxed β_{12} and GN sheets in the form of cif files.

For the relaxed β_{12} sheet:

```
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# CRYSTAL DATA
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_cell_length_c              19.995638
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_cell_angle_beta            90.000000
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_cell_volume                3559.034827
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_space_group_IT_number      1

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  'x, y, z'

loop_
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  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
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  B3          1.0      0.288221      0.252984      0.024911      Biso  1.000000 B
  B4          1.0      0.175698      0.252984      0.024910      Biso  1.000000 B
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  B6          1.0      0.233555      0.377989      0.024911      Biso  1.000000 B
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  B8          1.0      0.288221      0.502984      0.024911      Biso  1.000000 B
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  B14         1.0      0.175698      0.752984      0.024910      Biso  1.000000 B
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  B17         1.0      0.117864      0.877990      0.024911      Biso  1.000000 B
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For the relaxed GN sheet:

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_space_group_IT_number      1

loop_
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loop_
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  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
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