Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Improving Dioxin Sensing Properties of Graphene and Hexagonal Boron Nitride Based van der Waals Solids: A First-principles Study

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SI.1. Computational Details

The transport properties were calculated using TransSIESTA code implemented in SIESTA package, which is the combinations of NEGF within Keldysh formalism and DFT. The relaxations of atomic positions and electronic structure calculations were done by using double –ζ polarised numerical atomic orbital basis sets. The local density approximation and Troullier-Martin type norm-conserving pseudopotentials were used. A kinetic cutoff for real-space integral 200 Ry was used to expand the electron density. The convergence criteria for density matrix were chosen as 10^{-4} and 0.01 eV/Å for force tolerance. For calculating the transport properties, we have used 1×1×20 k meshes.

Two probe systems were considered with the scattering region sandwiched between semi-infinite left (source) and right (drain) electrodes. The landauer-Buttiker formula was used to calculate the current (I) passed through the systems at a finite bias voltage (V_b).

$$I(V_b) = G_0 \int_{\mu R}^{\mu L} T(E,V_b)dE$$

Where G_0= 2(e^2/h) is the unit of quantum conductance and T (E, V_b) is the transmission probability of electrons incident at an energy E through the device under the bias V_b. The chemical potential difference between the left and right electrode is e $V_b = \mu_L - \mu_R$.

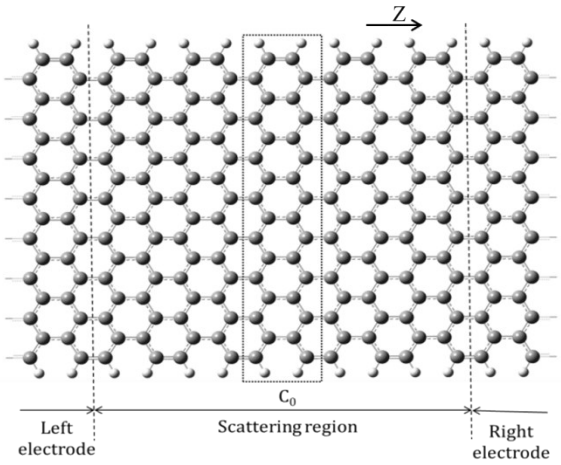
Table S1. Calculated Interlayer Distances and Bandgap of Homo and Hetero Bilayers of G and h-BN

	BLG	**BLBN**	**GBN**	**BNG**
Inter layer distance (Å)	3.31	3.16	3.16	3.16
Band gap (eV)	0	4.32	0.06	0.05

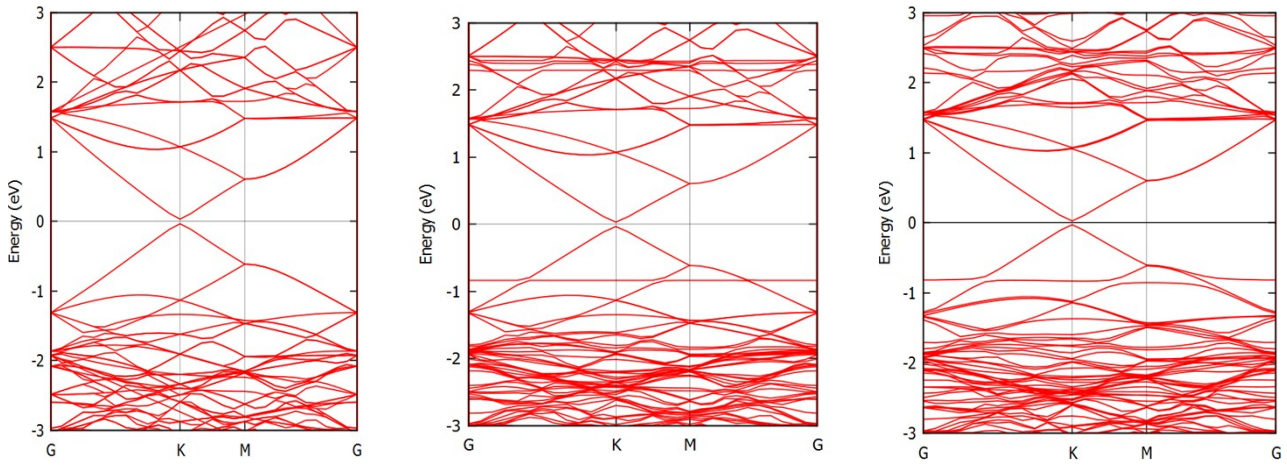
SI.2. Model Systems Used to Calculated the Transport Properties and I-V Characteristics

For calculating the transport properties, we have used 16 armchair nanoribbons for all the cases. For simplification, the naming of the systems was considered same as used in 2D sheets. The unit cell of scattering and electrode regions are same and they represented in dashed line in below **Scheme S1.** The lattice constant of the unit cell is C_0 and the scattering region is $5C_0$. In case of SLG (SLBN) nanoribbon, the electrode regions consists of 32

Carbon (16 Boron and 16 Nitrogen) atoms and 4 Hydrogen (4 H) atoms, and scattering region consist of 160 C (80 B and 80 N) atoms and 20 H (20H) atoms and in BLG (BLBN), the electrode region consist of 64 C (32 B and 32 N) and 8 H (8H) atoms and scattering regions consist of 320 C (160 B and 160 N) atoms and 40 H (40H) atoms. Similarly in the hetero bilayers (GBN and BNG) , the electrode regions consist of 32 C, 16 B , 16 N and 8 H atoms as well as the scattering region consist of 160 C, 80 B, 80 N and 40 H atoms. All the model system of TCDD interacted nanoribbons are shown in **Figure S4.**

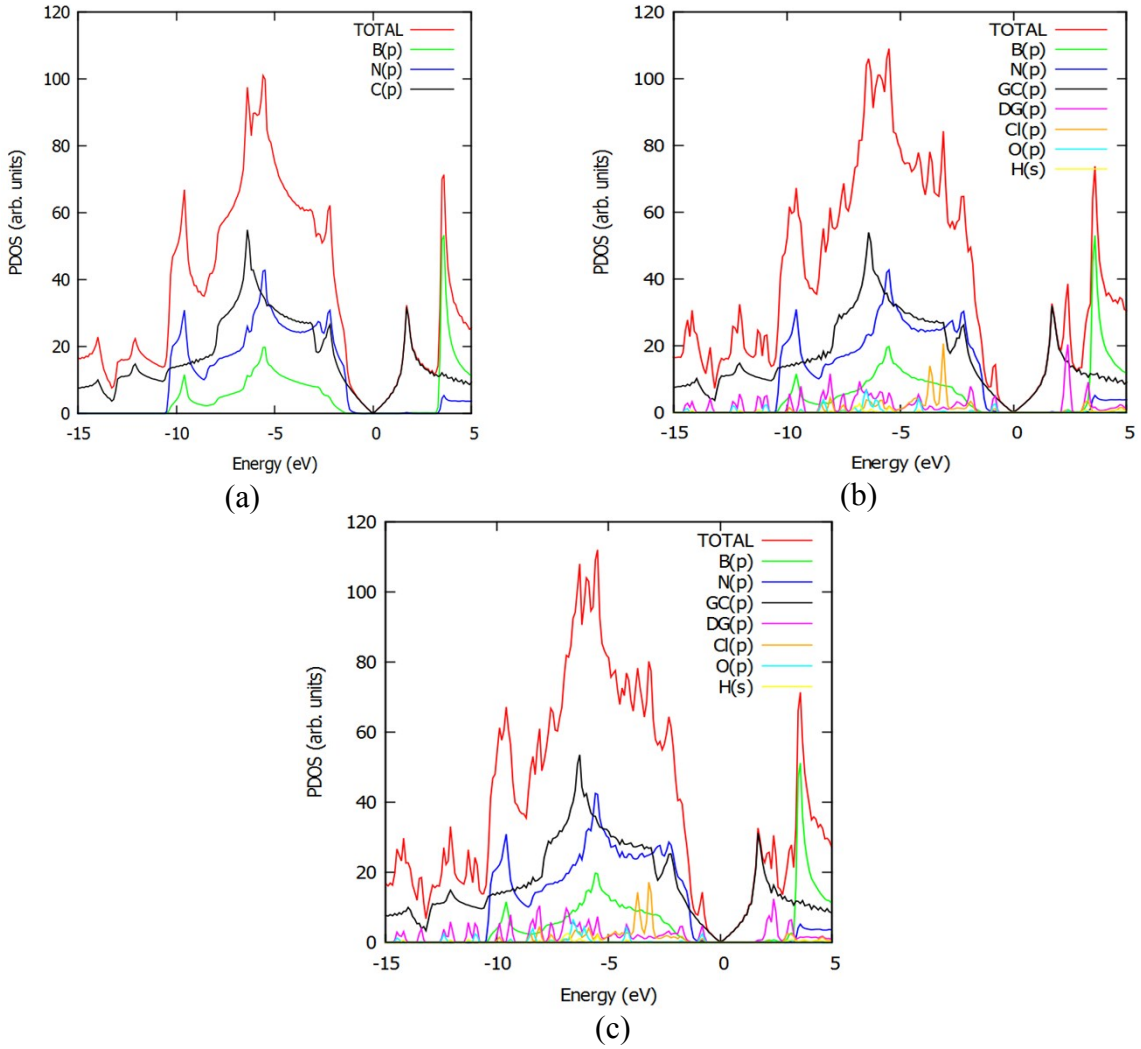


Scheme S1. Schematic model view of the two-probe armchair nanoribbon.



(a) (b) (c)

SI.Figure.S1. Band structures of (a) pristine GBN, (b) GBN-TCDD and (c) BNG-TCDD. The Fermi level was set to be zero.

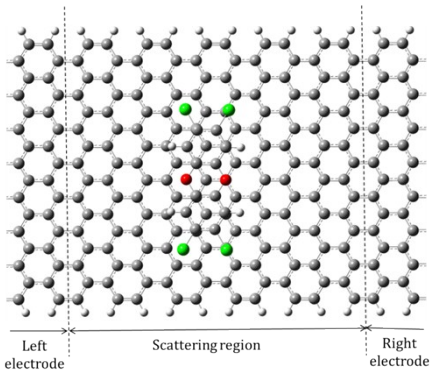


(a) (b)

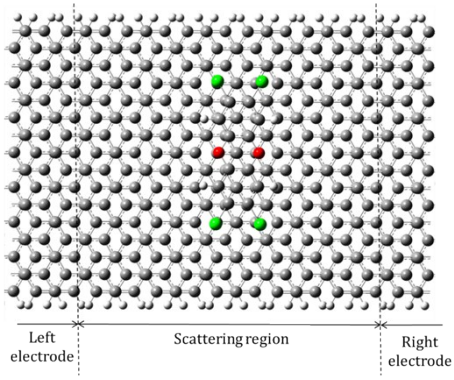
(c)

Figure S2. PDOS of (a) pristine GBN, (b) GBN-TCDD and (c) BNG-TCDD. The Fermi level was set to be zero

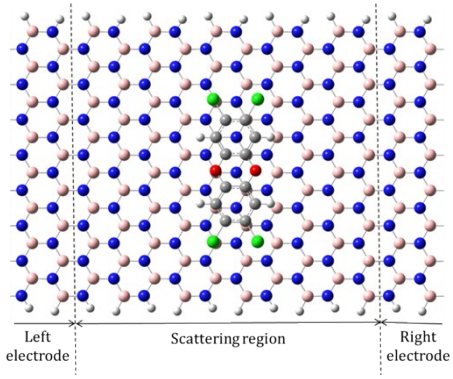
(a)


Left electrode
Scattering region
Right electrode

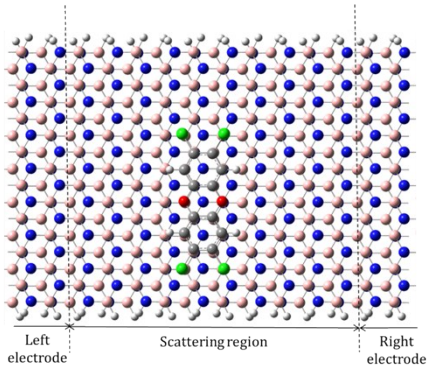
(b)


Left electrode
Scattering region
Right electrode

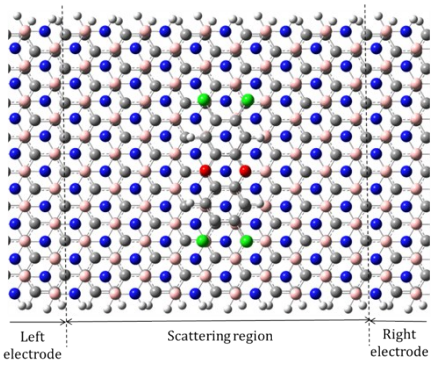
(c)


Left electrode
Scattering region
Right electrode

(d)


Left electrode
Scattering region
Right electrode

(e)



(f)

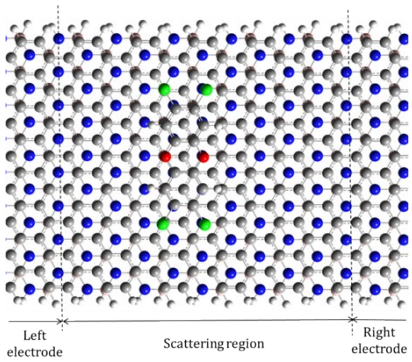
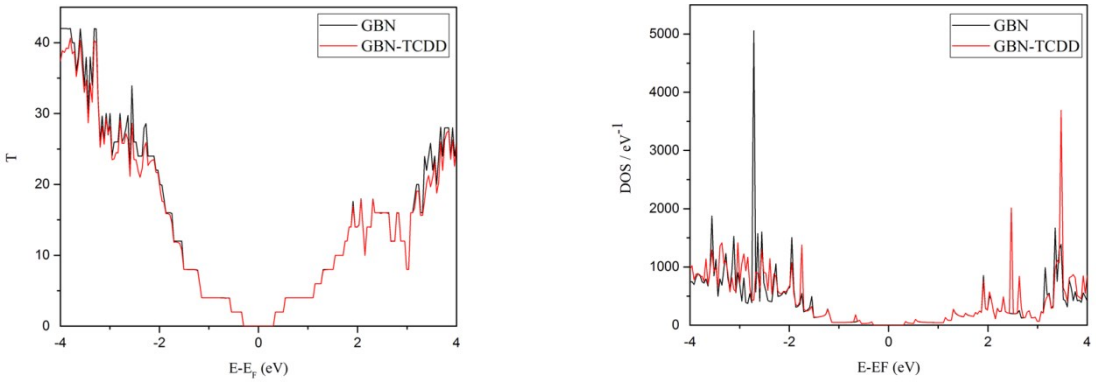
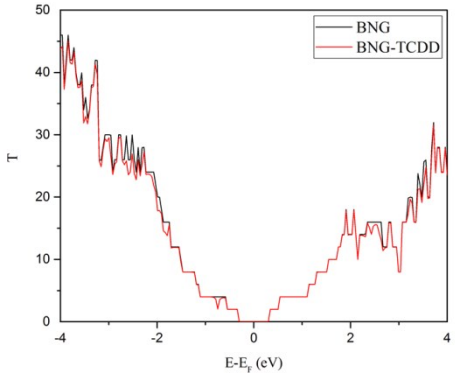


Figure S3. Model systems with TCDD used to calculate the transport properties. (a) SLG-TCDD (b) BLG-TCDD (c) SLBN-TCDD (d) BLBN-TCDD (e) GBN-TCDD and (f) BNG-TCDD.

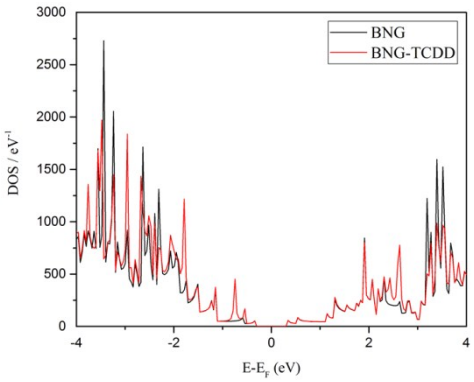


(a) (b)

Figure S4. Zero bias transmission spectra (a) and DOS (b) of GBN nanoribbon before and after interaction with TCDD.

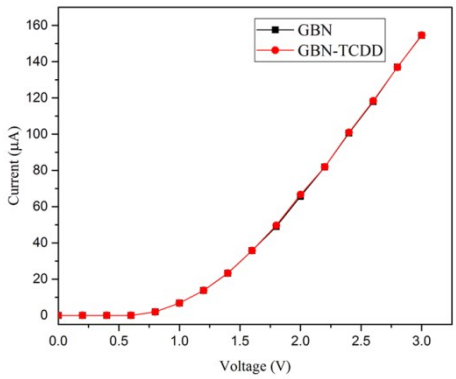


(a)

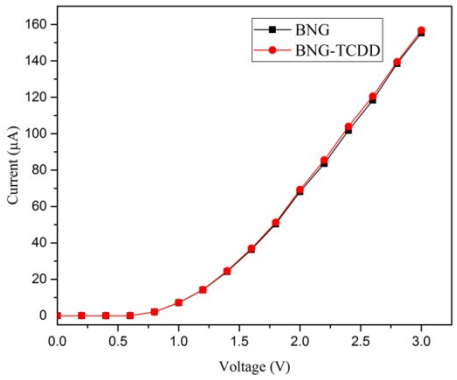


(b)

Figure S5. Zero bias transmission spectra (a) and DOS (b) of BNG nanoribbon before and after interaction with TCDD.



(a)



(b)

Figure S6. The Current-voltage (I-V) characteristics of pristine and TCDD adsorbed (a) GBN and (b) BNG nanoribbons

Table S2. Calculated Band Gap of 1D Armchair Nanoribbons Used in This Study

Systems	**E_g (eV)**	
	Pristine	**Complex**
SLG	0.68	0.66
BLG	0.38	0.38
SLBN	4.55	3.14
BLBN	4.34	3.02
GBN	0.62	0.61
BNG	0.62	0.62