Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Discriminating sensing of explosive molecules using graphene-boron nitride-graphene heteronanosheets

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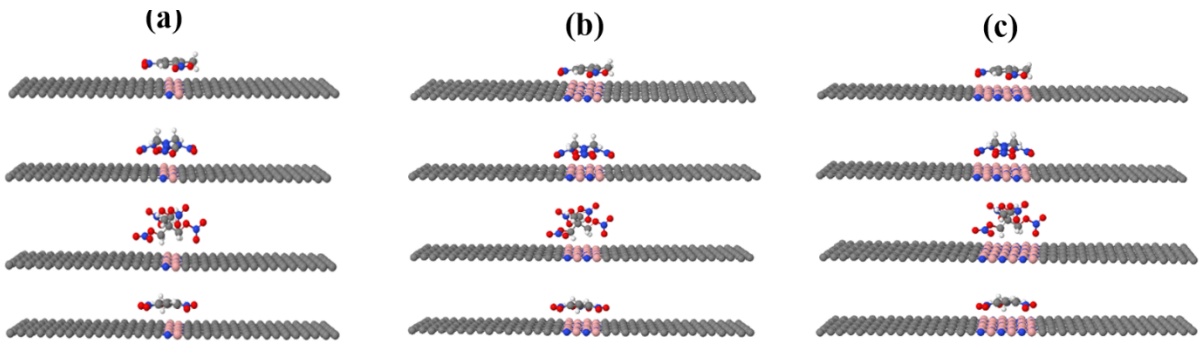

Figure S1: Shows the relaxed *h*-NSHs **(a)** with 1BN after place the DNT, HMX, PENT, and TNT molecules on the 1BN scatterer. **(b)** with 2BN after place the DNT, HMX, PENT, and TNT molecules on the 2BN scatterer. **(c)** with 3BN after place the DNT, HMX, PENT, and TNT molecules on the 3BN scatterer.

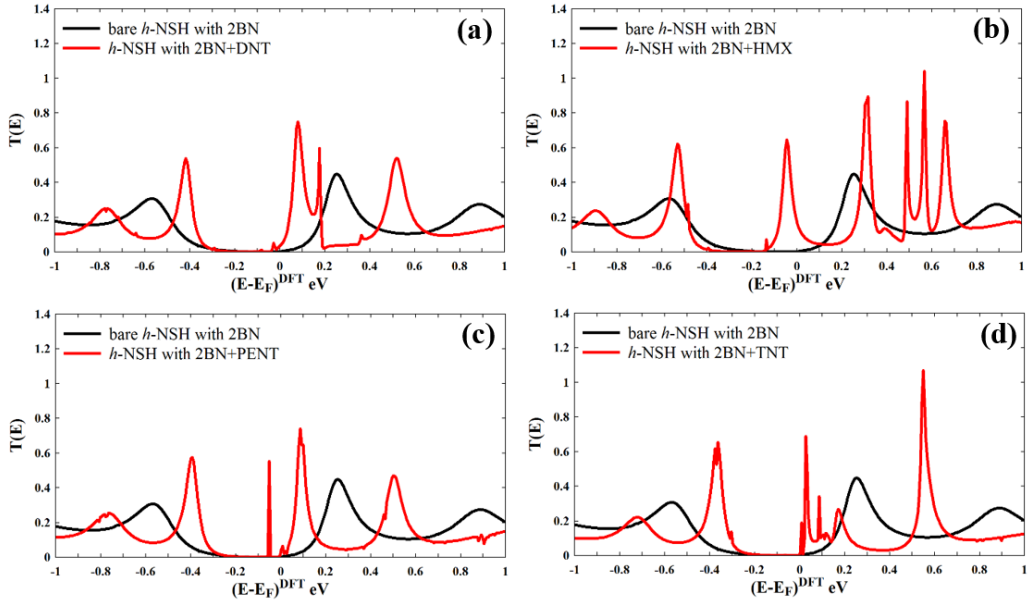

Figure S2: Shows the T(E) of the relaxed **(a)** *h*-NSH with 2BN+DNT, **(b)** *h*-NSH with 2BN+HMX, **(c)** *h*-NSH with 2BN+PENT, **(d)** *h*-NSH with 2BN+TNT. In all figures, the Fermi energy (E_F) is shifted at zero.

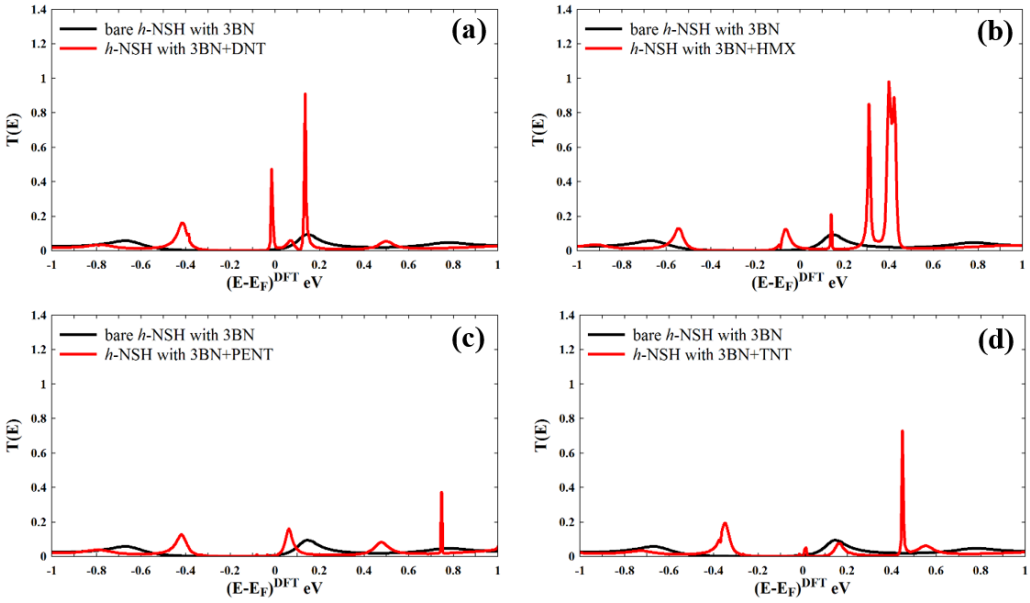

Figure S3: Shows the T(E) of the relaxed **(a)** *h*-NSH with 3BN+DNT, **(b)** *h*-NSH with 3BN+HMX, **(c)** *h*-NSH with 3BN+PENT, **(d)** *h*-NSH with 3BN+TNT. In all figures, the Fermi energy (E_F) is shifted at zero.

Table S1: Shows the values of the Seebeck coefficient of the *h*-NSHs with 1BN/2BN/3BN junctions before and after place the molecules.

***h*-NSH with 1BN**	**S ($\mu V/K$)**	***h*-NSH with 2BN**	**S ($\mu V/K$)**	***h*-NSH with 3BN**	**S ($\mu V/K$)**
bare	-185	bare	+39	bare	+138
+DNT	-242	+DNT	-175	+DNT	-24
+HMX	-96	+HMX	+72	+HMX	+83
+PENT	-278	+PENT	-146	+PENT	-176
+TNT	-214	+TNT	-113	+TNT	-73

To estimate the amount of charge transfer (CT), we performed the Mulliken charge analyses between the molecules and the *h*-NSH with 1BN/2BN/3BN as shown in table S2.

Table S2: The charge transfer (CT) between the *h*-NSH with 1BN/2BN/3BN and molecules (DNT, HMX, PENT and TNT), charge transfers are in electron per molecule.

Junction	**CT**			
	+DNT	**+HMX**	**+PENT**	**+TNT**
***h*-NSH with 1BN**	+ 0.110 *e*	+ 0.130 *e*	+ 0.120 *e*	+ 0.160 ***e***
***h*-NSH with 2BN**	+ 0.180 *e*	+ 0.210 *e*	+ 0.110 *e*	+ 0.140 *e*
***h*-NSH with 3BN**	+ **0.260** *e*	+ 0.210 *e*	+ 0.130 *e*	+ 0.203 *e*

Looking at the table S2, we can note that the obtained results show that the charge transfer is larger in *h*-NSH with 3BN+DNT compared to the *h*-NSH with 1BN, and *h*-NSH with 2BN.The positive sign means that the charge transferred from the *h*-NSH+1BN/2BN/3BN to the molecule [12, 62].