

Supplementary Information

NLO-Based Nitrobenzene Sensing Using Defective BN Nanosheets: A DFT Study

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Table S1: $E_{nanosheet}$ and $E_{NB\&nanosheet}$ (in a.u.) and adsorption energies (in kcal/mol) in the gas phase, calculated in B3LYP-D3/6-311G(d,p) theoretical level. E_{NB} is -436.89kcal/mol in this level.

	$E_{nanosheet}$	$E_{NB\&nanosheet}$	E_{ad}
BN-NB	-1925.81	-2362.71	-7.52
CB-NB	-1938.88	-2375.81	-25.62
CN-NB	-1909.00	-2345.91	-7.85
CBN-NB	-1922.16	-2359.07	-13.26
VB-NB	-1900.55	-2337.45	-10.22
VN-NB	-1870.72	-2307.64	-14.72

Table S2: $E_{nanosheet}$ and $E_{NB\&nanosheet}$ (in a.u.) and adsorption energies (in kcal/mol) in the water environment, calculated in B3LYP-D3/6-311G(d,p) theoretical level. E_{NB} is -436.90kcal/mol in this level.

	$E_{nanosheet}$	$E_{NB\&nanosheet}$	E_{ad}
BN-NB	-1925.82	-2362.73	-5.87
CB-NB	-1938.90	-2375.84	-28.09
CN-NB	-1909.02	-2345.92	-6.32
CBN-NB	-1922.18	-2359.08	-7.04
VB-NB	-1900.56	-2337.47	-7.34
VN-NB	-1870.74	-2307.66	-18.953

Table S3: $E_{nanosheet}$ and $E_{NB\&nanosheet}$ (in a.u.) and adsorption energies (in kcal/mol) in the gas phase, calculated in B3LYP/6-311G(d,p) theoretical level. E_{NB} is -436.86kcal/mol in this level.

	$E_{nanosheet}$	$E_{NB\&nanosheet}$	E_{ad}
BN-NB	-1925.61	-2362.48	-2.86
CB-NB	-1938.69	-2375.57	-9.82

CN-NB	-1908.81	-2345.67	-2.74
CBN-NB	-1921.96	-2358.83	-4.90
VB-NB	-1900.36	-2337.23	-2.65
VN-NB	-1870.53	-2307.40	-3.10

Table S4: $E_{nanosheet}$ and $E_{NB\&nanosheet}$ (in a.u.) and adsorption energies (in kcal/mol) in the water environment, calculated in B3LYP/6-311G(d,p) theoretical level. E_{NB} is -436.87kcal/mol in this level.

	$E_{nanosheet}$	$E_{NB\&nanosheet}$	E_{ad}
BN-NB	-1925.62	-2362.50	-2.20
CB-NB	-1938.70	-2375.59	-13.03
CN-NB	-1908.82	-2345.69	-2.05
CBN-NB	-1921.98	-2358.85	-2.22
VB-NB	-1900.37	-2337.25	-1.83
VN-NB	-1870.54	-2307.42	-4.08