**Supplementary File**

**ReaxFF based molecular dynamics simulations to explore the interfacial dynamics between defective h-BN nanosheet and water nanodroplets**

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**Figure S1.**2D h-BN nanosheet displacement in all the directions (x, y and z) with NPT ensemble and 300 K temperature (Y and X axis represent the displacement (in Å) and number of iterations, respectively)



**Figure S2.**2D h-BN nanosheet displacement in all the directions (x, y and z) with NPT ensemble and 800 K temperature (Y and X axis represent the displacement (in Å) and number of iterations, respectively)



**Figure S3.**2D defective h-BN nanosheet (with a boron vacancy) displacement in all the directions (x, y and z) with NPT ensemble and 300 K temperature (Y and X axis represent the displacement (in Å) and number of iterations, respectively)



**Figure S4.**2D defective h-BN nanosheet (with a nitrogen vacancy) displacement in all the directions (x, y and z) with NPT ensemble and 300 K temperature (Y and X axis represent the displacement (in Å) and number of iterations, respectively)



**Figure S5.** (a) Initial configuration showing a monolayer pristine h-BN nanosheet with water molecules around it, and (b) Final configuration showing the water molecules being accumulated at the surface of h-BN nanosheet [Yellow, blue, red and white coloured spheres correspond to boron, nitrogen, oxygen and hydrogen atoms, respectively]



**Figure S6.** Snapshots showing the vacancy defect in the h-BN monolayer of approximately area of (a) 30 Å2, and (b) 40 Å2 [Yellow and blue coloured spheres correspond to boron and nitrogen, respectively]

**Video S1.** Simulation displaying the water molecule dissociation and chemically adsorbing at the defected edge atoms of 2D h-BN nanosheet

**Video S2.** Simulation replicating the TGA experiment with water molecules and functionalized defected h-BN surface

**Table S1. Lattice parameters of h-BN and the BN bond length**

|  |  |  |
| --- | --- | --- |
| **h-BN lattice parameters** | | |
| **Experimental [1]** | **DFT [2]** | **ReaxFF [Present study]** |
| a=2.5040 Å and c=6.661 Å | a=2.5110 Å and c=6.679 Å | a=2.5219 Å and c=6.668 Å |
| **BN bond length in h-BN** | | |
| **Literature [3]** | **DFT [2]** | **ReaxFF [Present study]** |
| 1.450 Å | 1.450 Å | 1.451 Å |

**References:**

1. R.W. Lynch and H.G. Drickamer, Effect of high pressure on the lattice parameters of diamond, graphite, and hexagonal boron nitride, *The Journal of Chemical Physics*, 1966, 44, 181

2. M. Topsakal, E. Aktürk and S.J.P.R.B. Ciraci, First-principles study of two-and one-dimensional honeycomb structures of boron nitride, *Physical Review B*, 2009, 79, 115442

3. J. Wang, F. Ma and M. Sun, Graphene, hexagonal boron nitride, and their heterostructures: properties and applications, *RSC advances*, 2017, 7, 16801