

## Supplementary Material for

### An Efficient Way to Suppress the Competition Between Adsorption of H<sub>2</sub> and Desorption of nH<sub>2</sub>-Nb Complex from Graphene Sheet: A Promising Approach to H<sub>2</sub> Storage

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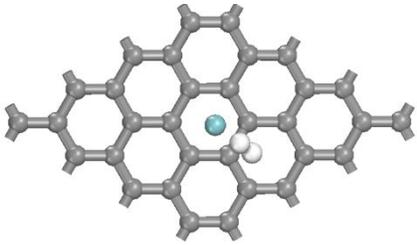
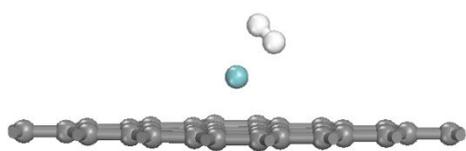
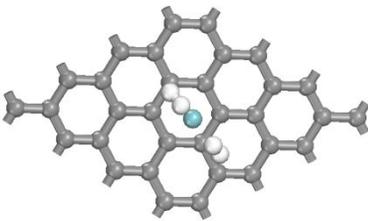
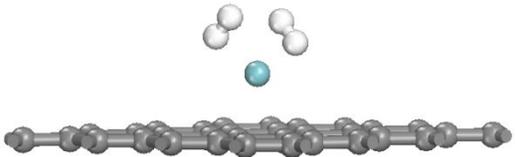
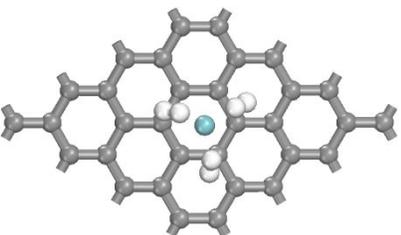
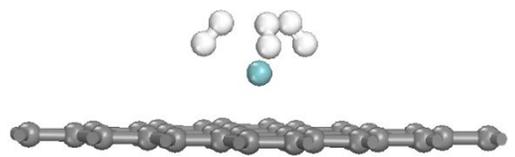
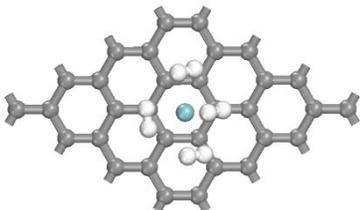
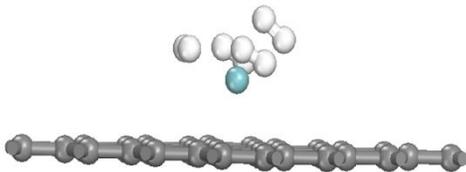
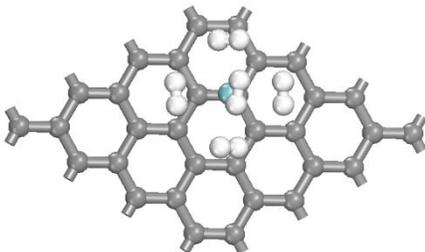
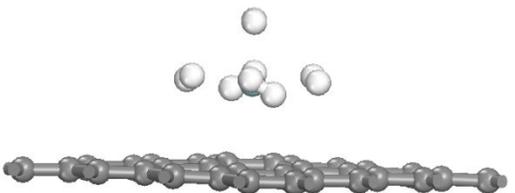
**Figure S1.** Side and Top views of the relaxed structures of the successive addition of H<sub>2</sub> adsorption on GR@Nb complex. The green balls represent the Nb atom, gray balls represent the C atoms and the white balls represent H atoms

**Figure S2.** Side and Top views of the relaxed structures of H<sub>2</sub> adsorption on NGR@2Nb complex. The green balls represent the Nb atom, gray balls represent the C atoms, blue represent N atom and the white balls represent H atoms

**Figure S3.** Projected density of states of pristine graphene (blue line), 2NGR@Nb complex (red line).and GR@Nb complex (green line).

**Figure S4.** Snapshots of MD of 2NGR@2Nb at 800K

**Figure S5.** Snapshots of MD simulations of 7H<sub>2</sub>-Nb at T=500K and 7H<sub>2</sub>-2NGR@Nb at T=600K.

Number of H <sub>2</sub>	Side view of nH <sub>2</sub> -GR@2Nb	Top view of nH <sub>2</sub> -GR@2Nb
1		
2		
3		
4		
5		

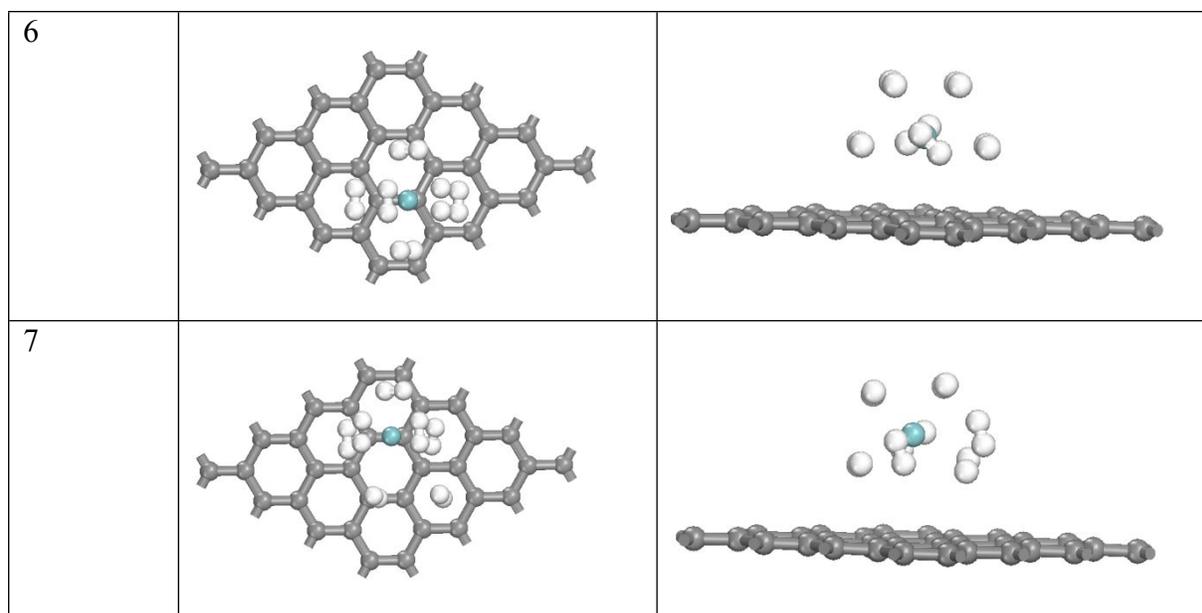
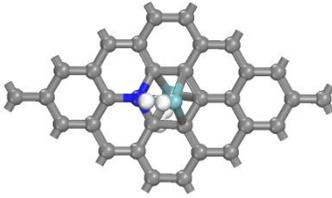
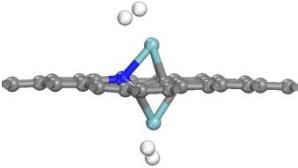
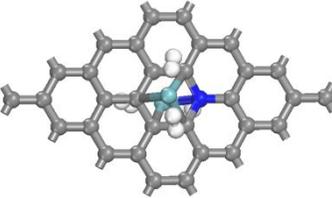
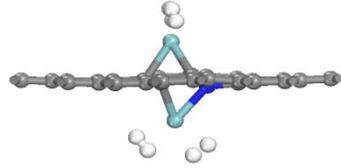
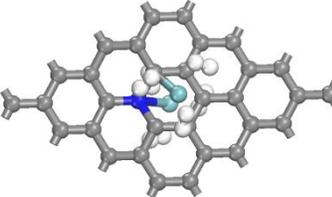
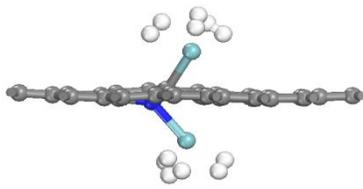
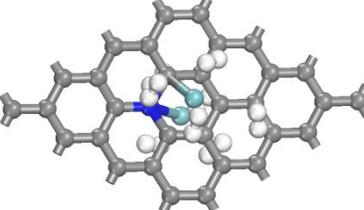
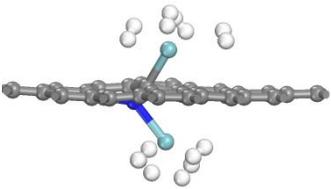
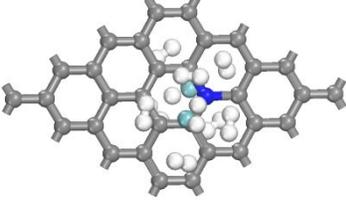
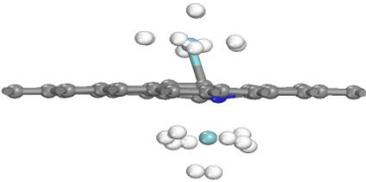
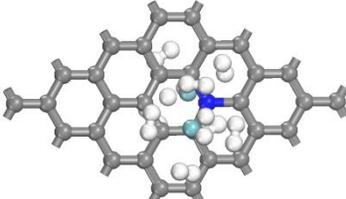
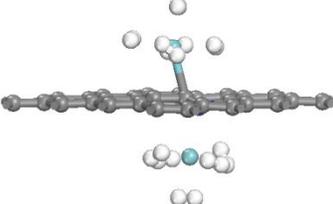
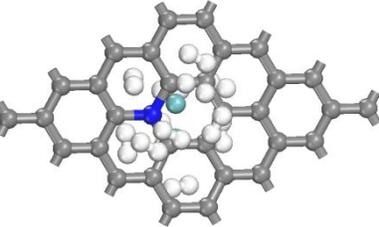
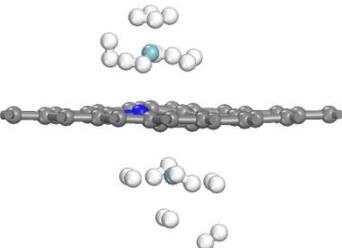


Figure S1. Side and Top views of the relaxed structures of the successive addition of H<sub>2</sub> adsorption on GR@Nb complex. The green balls represent the Nb atom, gray balls represent the C atoms and the white balls represent H atom

Number of H <sub>2</sub>	E <sub>b</sub> (eV)	Side view of nH <sub>2</sub> -NGR@2Nb	Top view of nH <sub>2</sub> -NGR@2Nb
2H <sub>2</sub>	0.637	 A side view of a nanographene ring (NGR) with two hydrogen molecules (H2) adsorbed on its surface. The NGR is shown as a gray carbon lattice. The H2 molecules are represented by two white spheres (hydrogen) and one cyan sphere (nitrogen) bonded to the carbon lattice.	 A top view of the NGR@2Nb system. The NGR is a horizontal gray chain. Two H2 molecules are adsorbed on the top and bottom surfaces, each shown as a cyan sphere bonded to the chain with two white spheres.
4H <sub>2</sub>	0.652	 A side view of a nanographene ring (NGR) with four hydrogen molecules (H2) adsorbed on its surface. The NGR is shown as a gray carbon lattice. The H2 molecules are represented by two white spheres (hydrogen) and one cyan sphere (nitrogen) bonded to the carbon lattice.	 A top view of the NGR@4Nb system. The NGR is a horizontal gray chain. Four H2 molecules are adsorbed on the top and bottom surfaces, each shown as a cyan sphere bonded to the chain with two white spheres.
6H <sub>2</sub>	0.632	 A side view of a nanographene ring (NGR) with six hydrogen molecules (H2) adsorbed on its surface. The NGR is shown as a gray carbon lattice. The H2 molecules are represented by two white spheres (hydrogen) and one cyan sphere (nitrogen) bonded to the carbon lattice.	 A top view of the NGR@6Nb system. The NGR is a horizontal gray chain. Six H2 molecules are adsorbed on the top and bottom surfaces, each shown as a cyan sphere bonded to the chain with two white spheres.
8H <sub>2</sub>	0.580	 A side view of a nanographene ring (NGR) with eight hydrogen molecules (H2) adsorbed on its surface. The NGR is shown as a gray carbon lattice. The H2 molecules are represented by two white spheres (hydrogen) and one cyan sphere (nitrogen) bonded to the carbon lattice.	 A top view of the NGR@8Nb system. The NGR is a horizontal gray chain. Eight H2 molecules are adsorbed on the top and bottom surfaces, each shown as a cyan sphere bonded to the chain with two white spheres.

10H <sub>2</sub>	0.561		
12H <sub>2</sub>	0.46		
14H <sub>2</sub>	0.397		

**Figure S2.** Side and Top views of the relaxed structures of H<sub>2</sub> adsorption at 3.6% concentration of N atoms (NGR@2Nb) complex. The green balls represent the Nb atom, gray balls represent the C atoms, blue represent N atom and the white balls represent H atoms

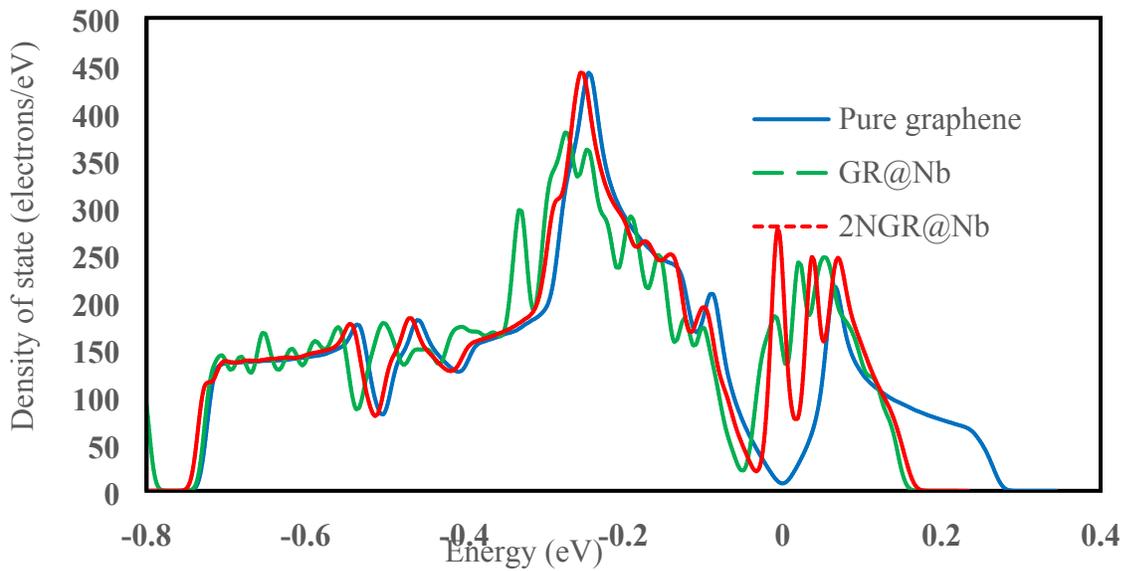


Figure S3 Projected density of states of pristine graphene (blue line), 2NGR@Nb complex (red line) and GR@Nb complex (green line).

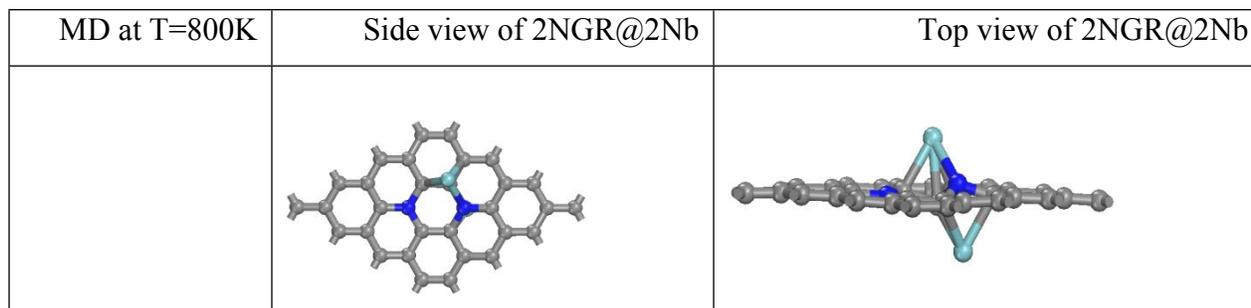


Figure S4 Snapshots of MD of 2NGR@2Nb at 800K

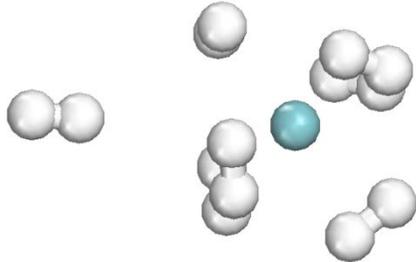
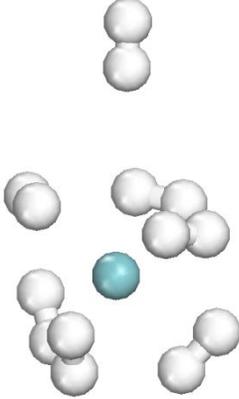
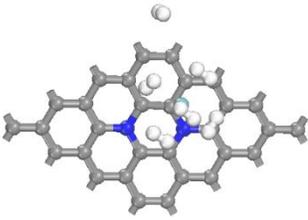
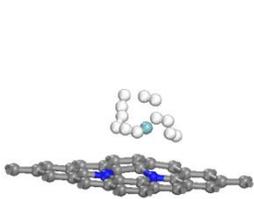
MD simulation	Side view	Top view
Case(a) $7\text{H}_2\text{-Nb}$ complex  $T=500\text{K}$		
Case(b) $7\text{H}_2\text{-2NGR@Nb}$ complex  $T=600\text{K}$		

Figure S5 Snapshots of MD simulations of  $7\text{H}_2\text{-Nb}$  at  $T=500\text{K}$  and  $7\text{H}_2\text{-2NGR@Nb}$  at  $T=600\text{K}$ .