Supplementary Material for

An Efficient Way to Suppress the Competition Between Adsorption of H_2 and Desorption of nH_2-Nb Complex from Graphene Sheet: A Promising Approach to H_2 Storage

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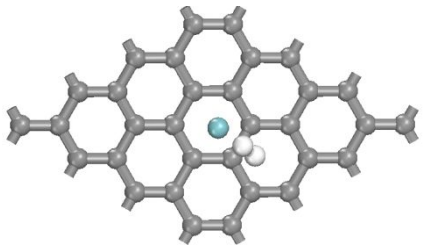
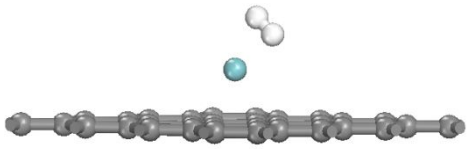
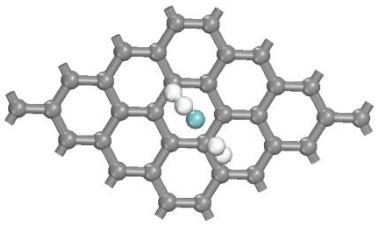
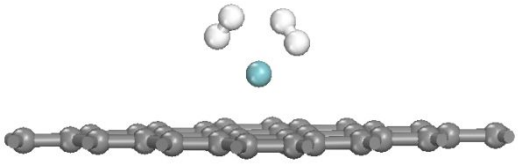
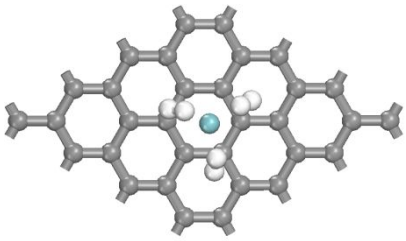
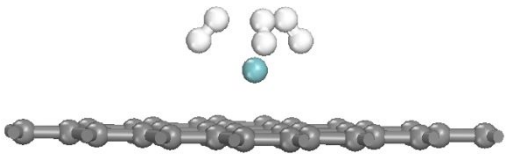
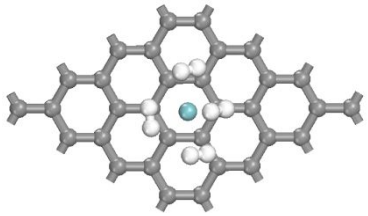
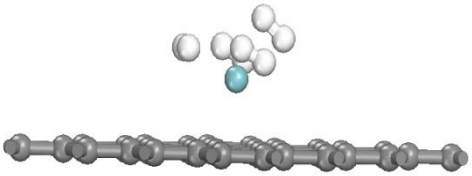
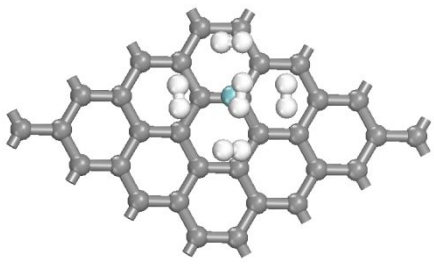
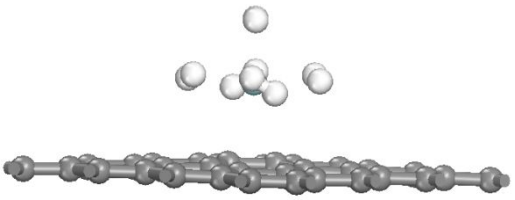
Number of H_2	Side view of nH_2-GR@2Nb	Top view of nH_2-GR@2Nb
1		
2		
3		
4		
5		

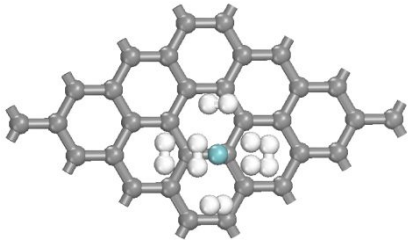
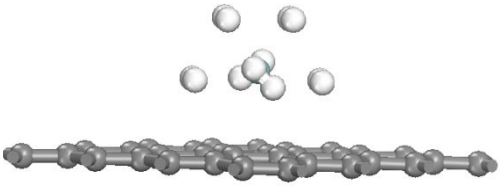
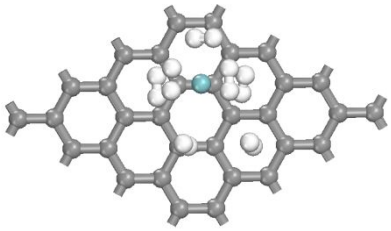
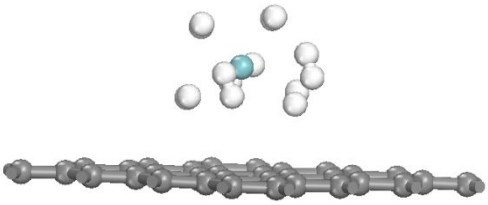
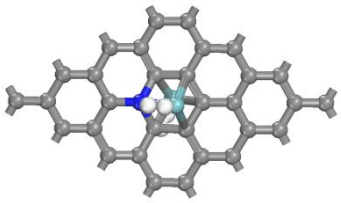
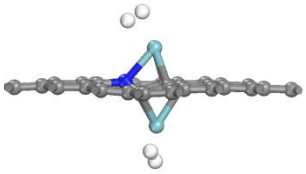
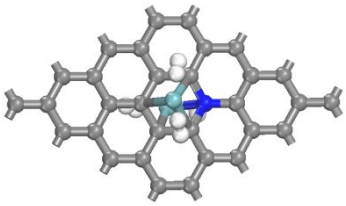
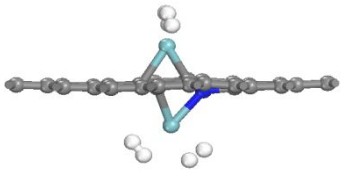
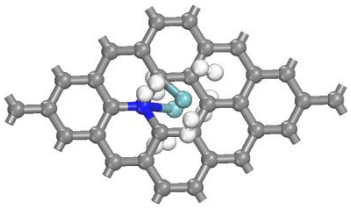
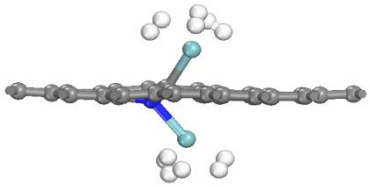
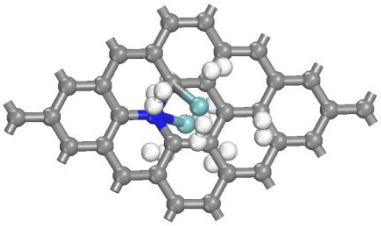
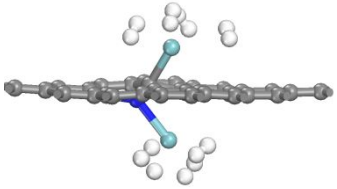
6		
7		

Figure S1.Side and Top views of the relaxed structures of the successive addition of H_2 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_2	Eb(eV)	Side view of nH_2-NGR@2Nb	Top view of nH_2-NGR@2Nb
$2H_2$	0.637		
$4H_2$	0.652		
$6H_2$	0.632		
$8H_2$	0.580		

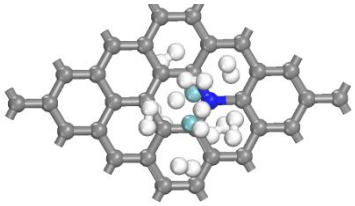
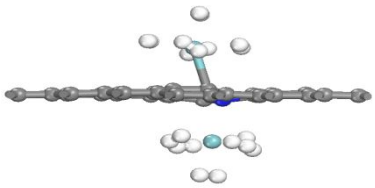
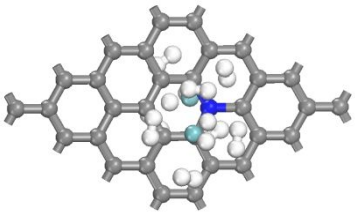
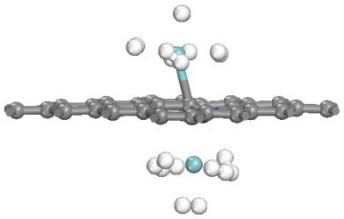
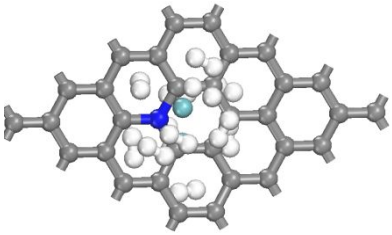
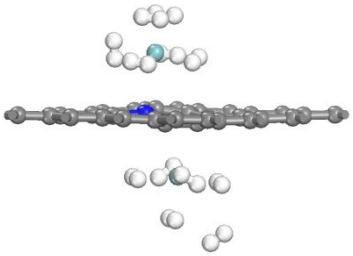
$10H_2$	0.561		
$12H_2$	0.46		
$14H_2$	0.397		

Figure S2.Side and Top views of the relaxed structures of H_2 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

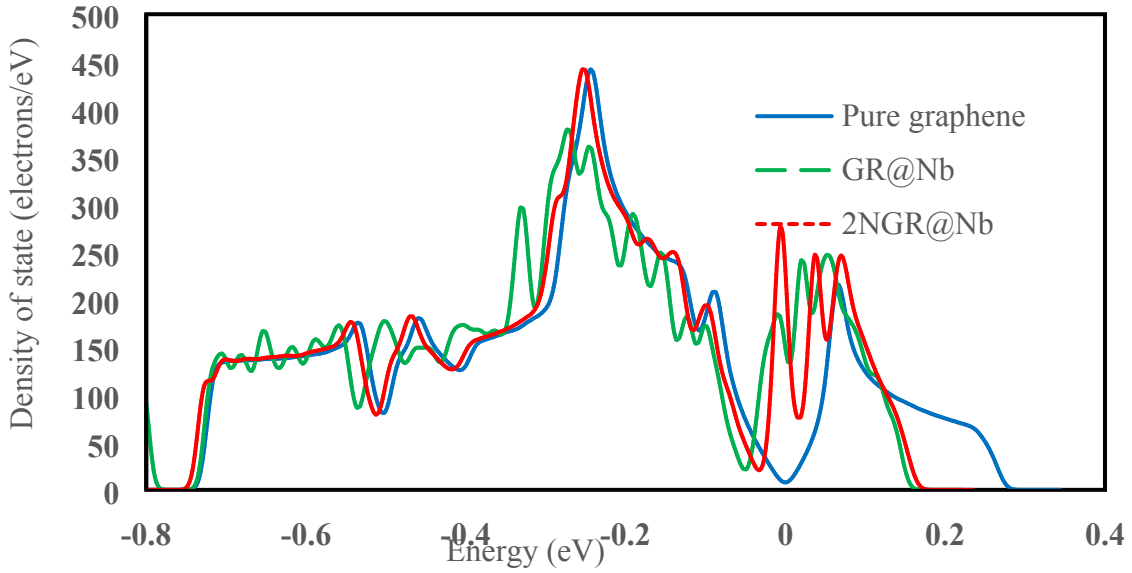


Figure S3 Projected density of states of pristine graphene (blue line), 2NGR@Nb complex (red line).and GR@Nb complex (green line).

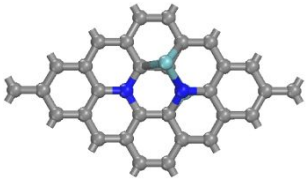
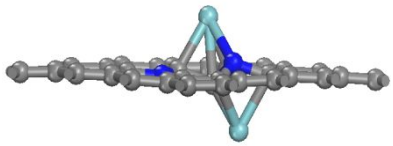
MD at T=800K	Side view of 2NGR@2Nb	Top view of 2NGR@2Nb
		

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

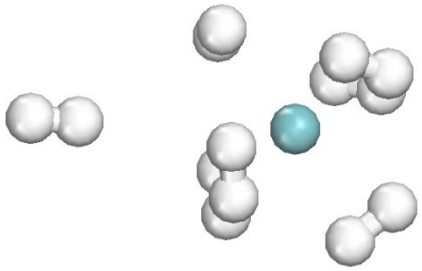
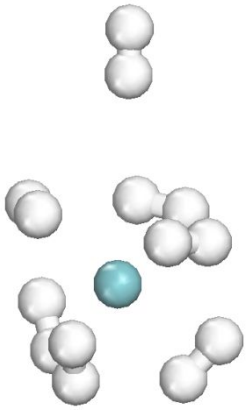
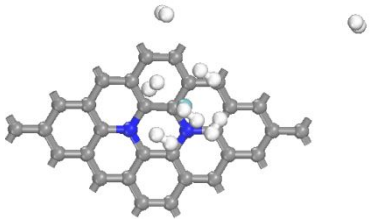
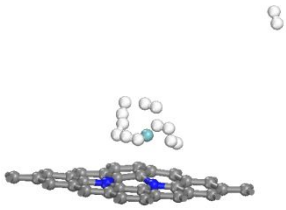
MD simulation	Side view	Top view
Case(a) 7H_2-Nb complex T=500K		
Case(b) 7H_2-2NGR@Nb complex T=600K		

Figure S5 Snapshots of MD simulations of 7H_2-Nb at T=500K and 7H_2-2NGR@Nb at T=600K.