Supporting Information

Niobium Decorated 2D Biphenylene as High-Capacity Hydrogen Storage Material: Combined DFT and AIMD Simulations

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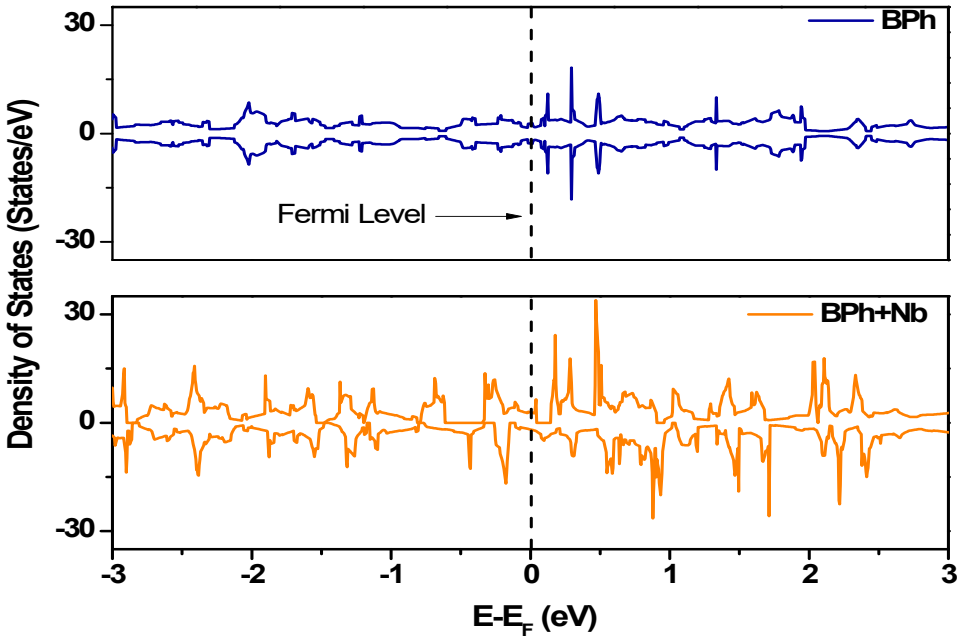

Figure S1: Total Density of States (TDOS) plot for BPh (upper panel)and BPh+Nb (lower panel). Here, the fermi level is set to 0eV and is denoted by a dotted line. The x and y axes indicate Energy (eV) and Density of States (States /eV)

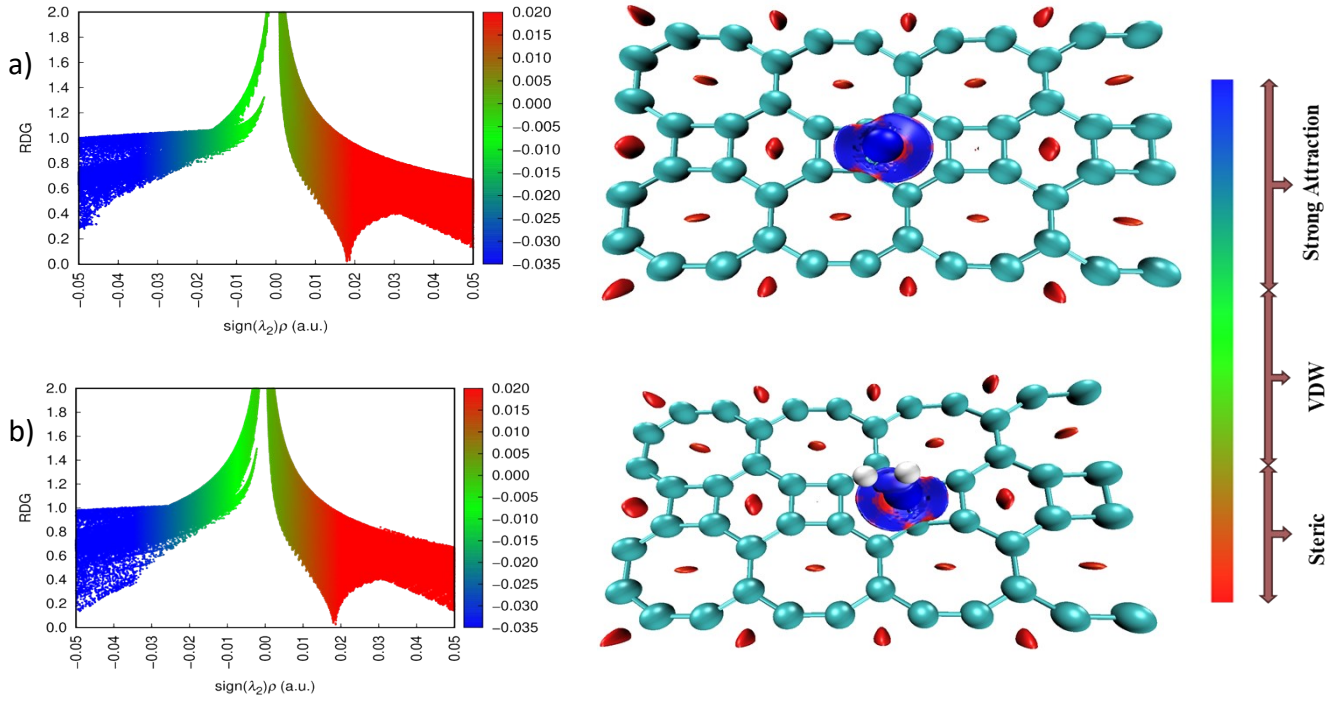

Figure S2: RDG scatter plots for a) BPh+Nb and b) BPh+Nb+1H_2 systems

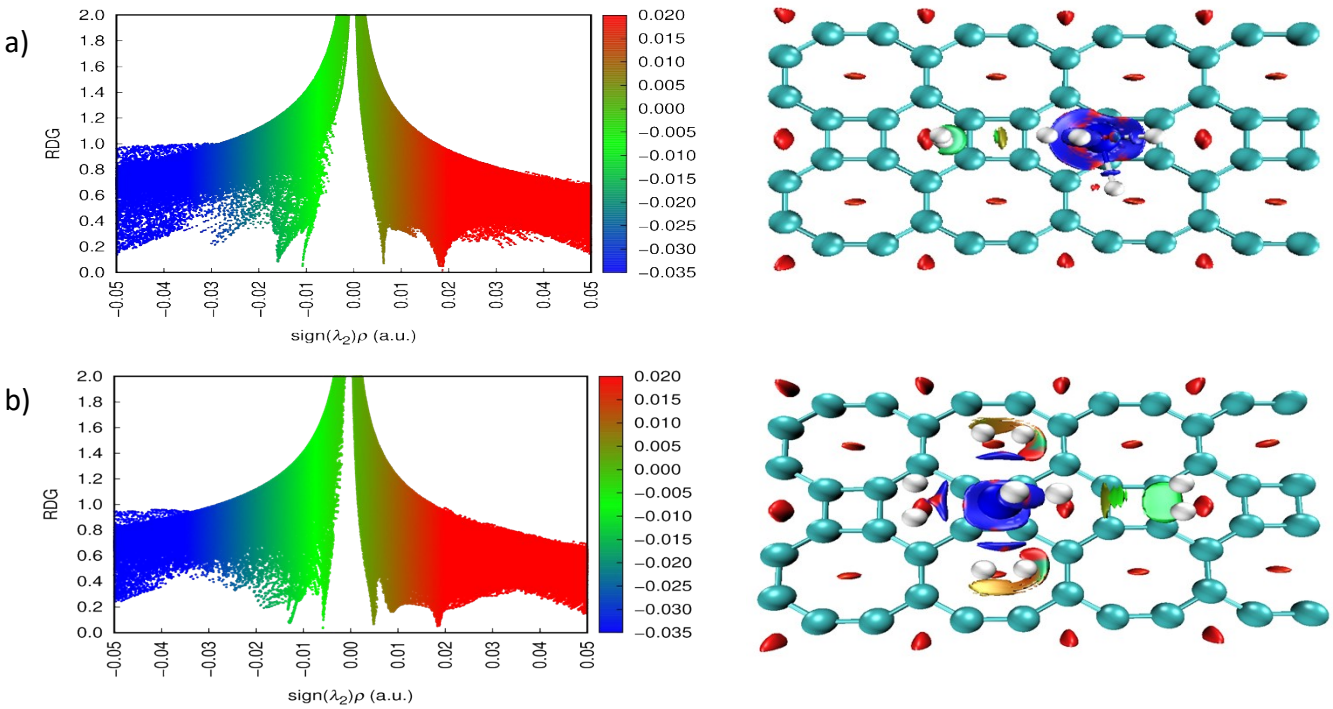

Figure S3: RDG scatter plots for a) BPh+Nb+ 3H_2 and b) BPh+Nb+5H_2 systems

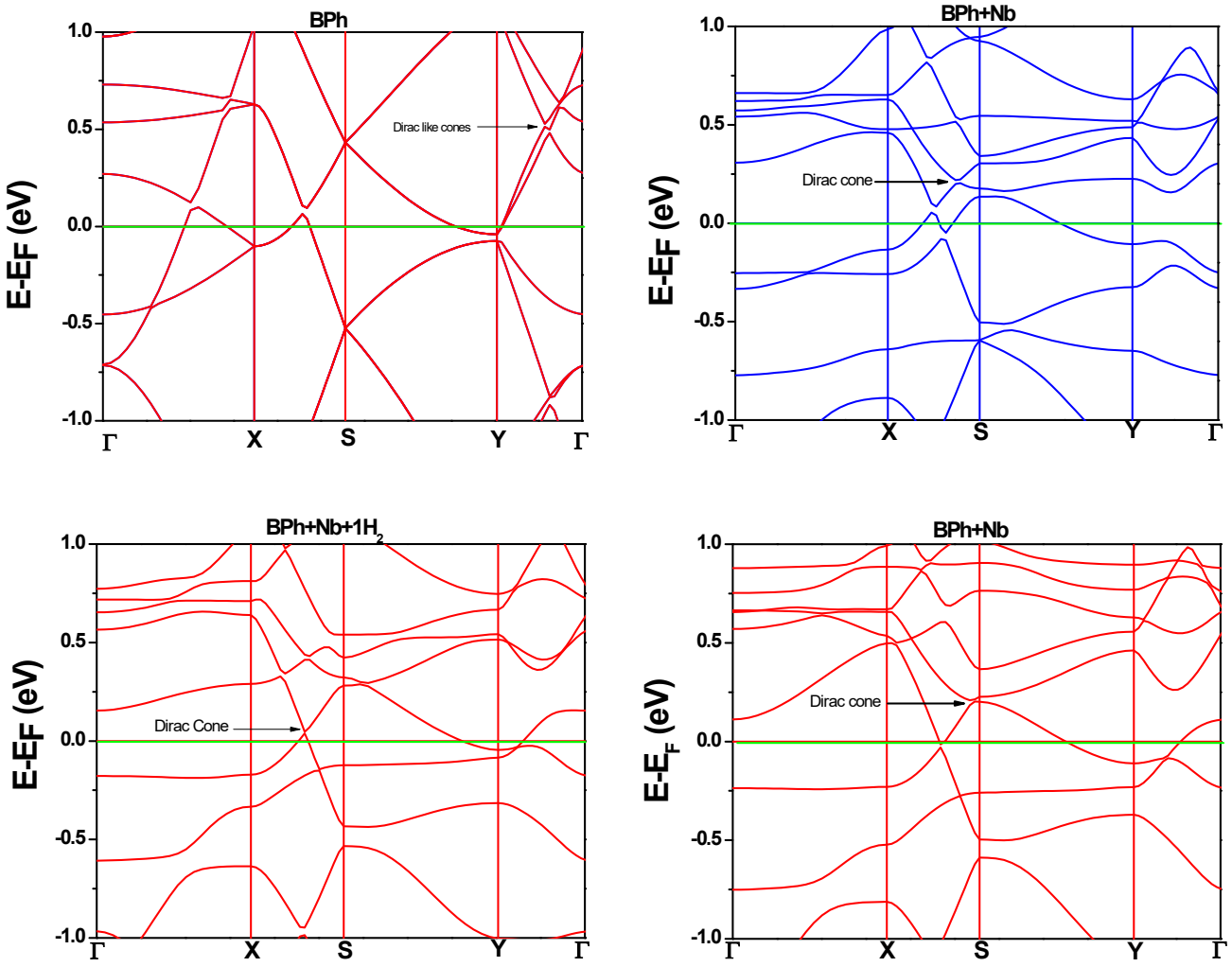

Figure S4: Band structure plot of pristine BPh, BPh+Nb and BPh+Nb+1H_2 with Dirac like cones. (Red, blue and green color indicates spin-up, spin down states and fermi level respectively)

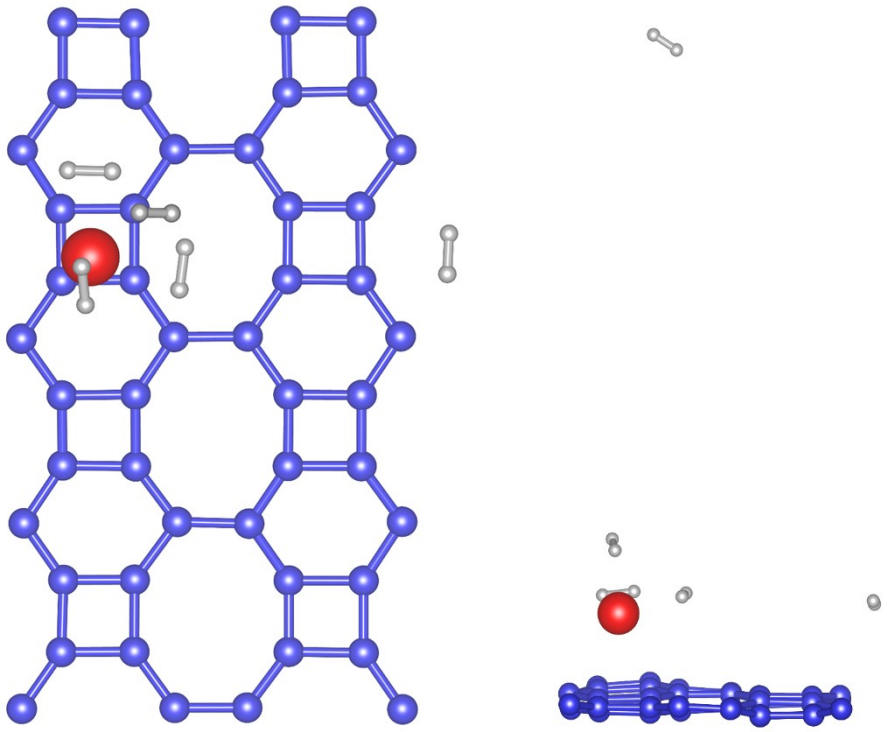

Figure S5: AIMD profile of BPh+Nb+5H_2 after 10 ps and a timestep of 1 fs at ambient conditions

Table S1: Vacuum Potential and Work functions for the systems, BPh, BPh+ Nb and BPh+Nb+1H_2

System	Vacuum Potential(eV)	Work Function(eV)
BPh	0.82	4.17
BPh+ Nb	0.96	3.87
BPh+ Nb+ 1H_2	1.05	4.19

Table S2: Comparison of Hydrogen storage capacity of BPh-Nb system with other nanomaterials

Material	**Hydrogen Uptake Capacity**	**Eads(eV/H_2)**	**Desorption Temperature (K)**	**References**
1Ti.C468	6.713%	−0.199	523.052	[67]
Zr-BPh	9.95%	−0.4	—	[32]
Nb-planar circumcoronene	—	−0.61	—	[68]
Nb@αGe	6.11%	−0.43	—	[79]
Nb- (h-BN)	—	−0.65	—	[68]
Nb-(C6/h − BN)	—	−0.58	—	[68]
2NGR@2Nb	8 %	0.465	344	[73]
4Li@BN-BPh/C-BPh	6.44%	−0.306	—	[69]
I-BPh	10.78%	—	—	[70]
Ca-BPh	6.66%	−0.23	280	[71]
Sc-BPh	6.40%	−0.33	370	[71]
V-BPh	7.52 %	−0.51	595.96	[72]
Y@CNF	—	-0.108	—	[81]
Zr@CNF	—	-0.081	—	[81]
Nb@CNF	—	-0.072	—	[81]
Nb-BPh (present work)	**5.76%**	**−0.61**	**380**	**—**

Table S3: Average C-Nb distance with corresponding Binding energy for BPh+ Nb system with addition of H_2

System	C-Nb Distance (Å)	BE (eV)
BPh+ Nb	2.15	—
BPh+ Nb+ $1H_2$	2.17	-0.69
BPh+ Nb+ $3H_2$	2.18	-0.69
BPh+ Nb+ $5H_2$	2.27	-0.46