Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Anodic voltage performance of conducting polymer-functionalized boron nitride nanosheets: A DFT assessment

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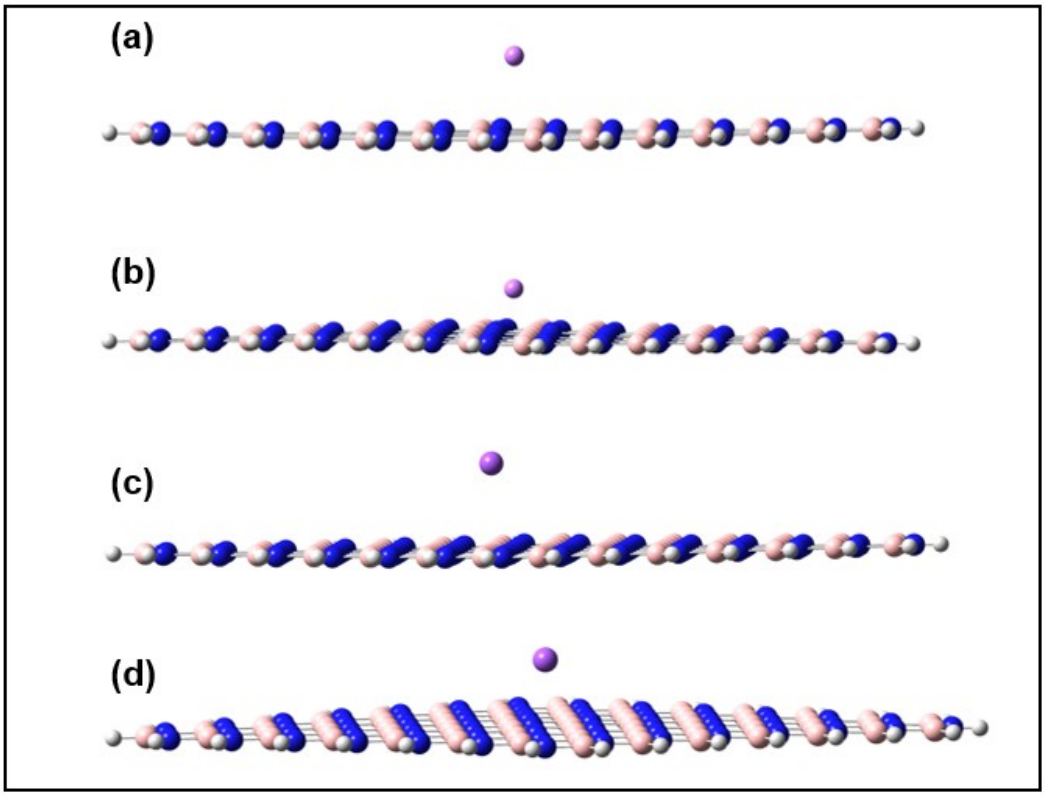


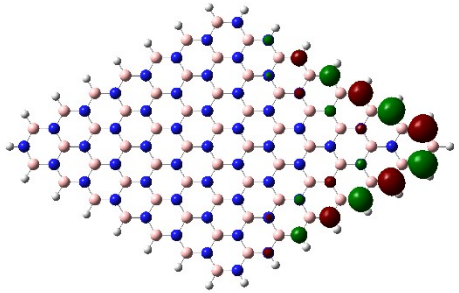
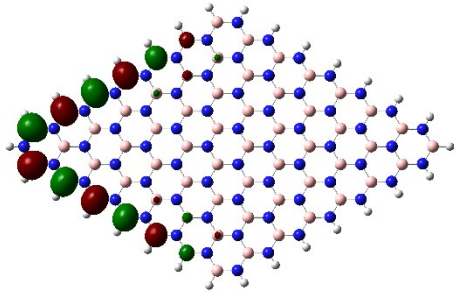
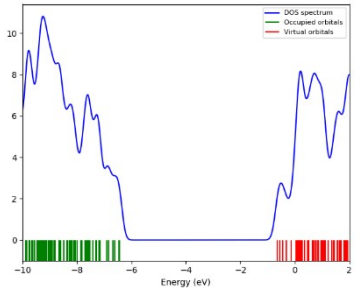
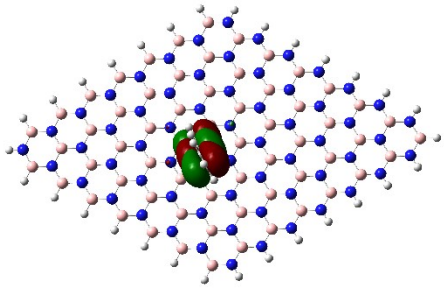
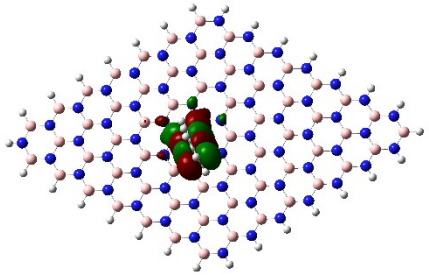
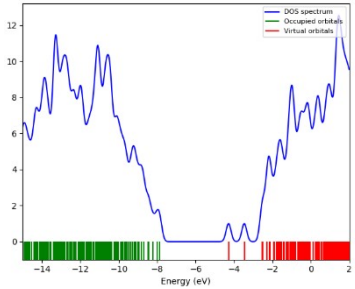
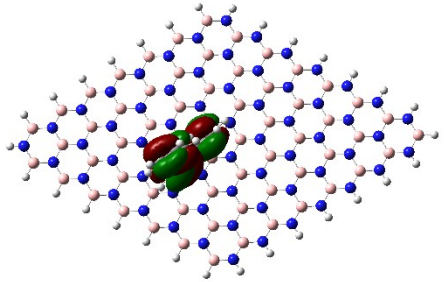
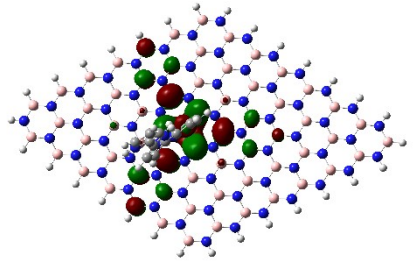
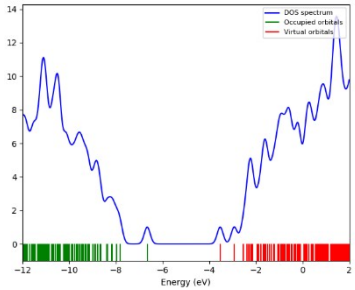
Figure S1. Optimized cross-sectional structures of (a) Li@BNNS (b) Li^{+}@BNNS, (c) Na@BNNS, and (d) Na^{+}@BNNS. The pristine boron nitride nanosheet (BNNS) comprises 63 atoms of boron and nitrogen each with tangling atoms at the structural boundaries saturated with hydrogen atoms to minimize the boundary effects [37].

Table S1. Adsorption distances of metals and metal-ions on BNNS complexes.

BNNS	Li@BNNS	Li^+@BNNS	Na@BNNS	Na^+@BNNS
B-N Bond Distance (Å)				
1.45	1.45	1.46	1.45	1.46
M/M^{n+}-N Bond Distance (Å)				
0.00	3.31	2.23	3.66	2.73
M/M^{n+}-B Bond Distance (Å)				
0.00	3.33	2.33	3.91	2.80

Table S2. Adsorption distances of conducting polymers, metals, and metal-ions on BNNS and CP-BNNS complexes.

B-N Bond Distance (Å)											
PA-BNNS	**PA-BNNS**	**Li@PA-BNNS**	**Li^+@PA-BNNS**	**Na@PA-BNNS**	**Na^+@PA-BNNS**	**PP-BNNS**	**PP-BNNS**	**Li@PP-BNNS**	**Li^+@PP-BNNS**	**Na@PP-BNNS**	**Na^+@PP-BNNS**
	1.55	1.48	1.48	1.48	1.48		1.56	1.45 (float)	1.48	1.45 (float)	1.48
PPPh-BNNS	**PPPh-BNNS**	**Li@PPPh-BNNS**	**Li^+@PPPh-BNNS**	**Na@PPPh-BNNS**	**Na^+@PPPh-BNNS**	**PT-BNNS**	**PT-BNNS**	**Li@PT-BNNS**	**Li^+@PT-BNNS**	**Na@PT-BNNS**	**Na^+@PT-BNNS**
	1.56	1.46(float)	1.48	1.45(float)	1.48		1.56	1.46(float)	1.49	1.45(float)	1.48
M/M^{n+}-N Bond Distance (Å)											
PA-BNNS	**PA-BNNS**	**Li@PA-BNNS**	**Li^+@PA-BNNS**	**Na@PA-BNNS**	**Na^+@PA-BNNS**	**PP-BNNS**	**PP-BNNS**	**Li@PP-BNNS**	**Li^+@PP-BNNS**	**Na@PP-BNNS**	**Na^+@PP-BNNS**
	-	2.97	2.36	2.85	2.71		-	2.83	2.60	2.63	2.77
PPPh-BNNS	**PPPh-BNNS**	**Li@PPPh-BNNS**	**Li^+@PPPh-BNNS**	**Na@PPPh-BNNS**	**Na^+@PPPh-BNNS**	**PT-BNNS**	**PT-BNNS**	**Li@PT-BNNS**	**Li^+@PT-BNNS**	**Na@PT-BNNS**	**Na^+@PT-BNNS**
	-	2.32	2.28	2.74	2.92		-	3.15	2.22	2.75	2.79
M/M^{n+}-B Bond Distance (Å)											
PA-BNNS	**PA-BNNS**	**Li@PA-BNNS**	**Li^+@PA-BNNS**	**Na@PA-BNNS**	**Na^+@PA-BNNS**	**PP-BNNS**	**PP-BNNS**	**Li@PP-BNNS**	**Li^+@PP-BNNS**	**Na@PP-BNNS**	**Na^+@PP-BNNS**
	-	2.58	2.46	2.91	2.83		-	2.68	2.45	3.04	2.90
PPPh-BNNS	**PPPh-BNNS**	**Li@PPPh-BNNS**	**Li^+@PPPh-BNNS**	**Na@PPPh-BNNS**	**Na^+@PPPh-BNNS**	**PT-BNNS**	**PT-BNNS**	**Li@PT-BNNS**	**Li^+@PT-BNNS**	**Na@PT-BNNS**	**Na^+@PT-BNNS**
	-	2.40	2.39	2.67	3.02		-	2.69	2.68	2.94	2.86

	HOMO	LUMO	DOS
BNNS			
PA-BNNS			
PP-BNNS			

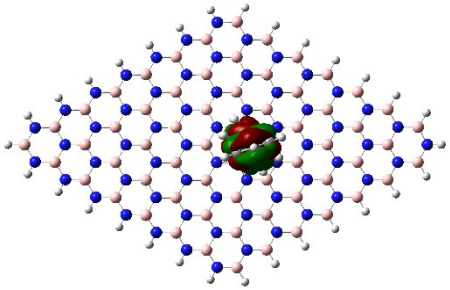
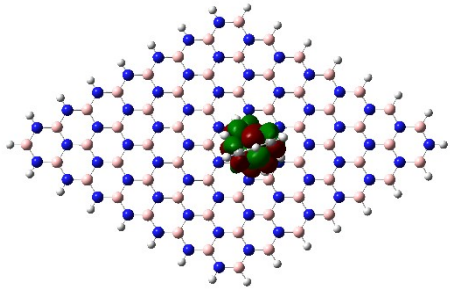
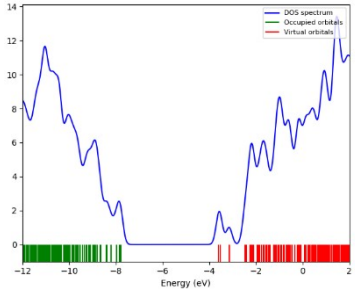
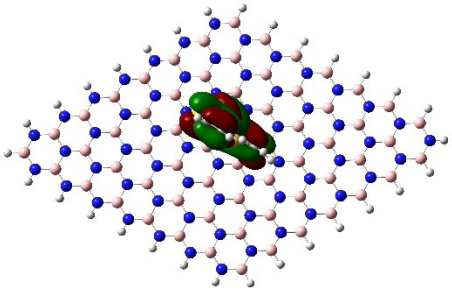
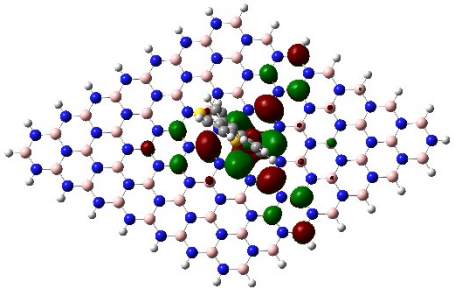
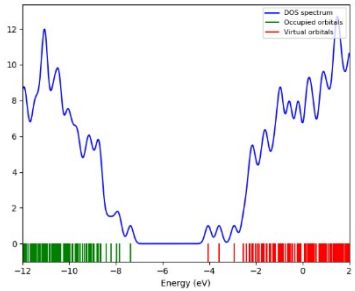
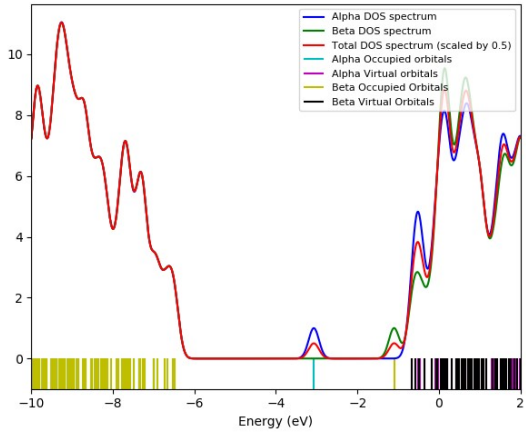
PPPh-BNNS			
PT-BNNS			

Figure S2. The HOMO and LUMO iso-surfaces of the conducting polymers adsorbed onto the BNNS (M/Mn+@BNNS).

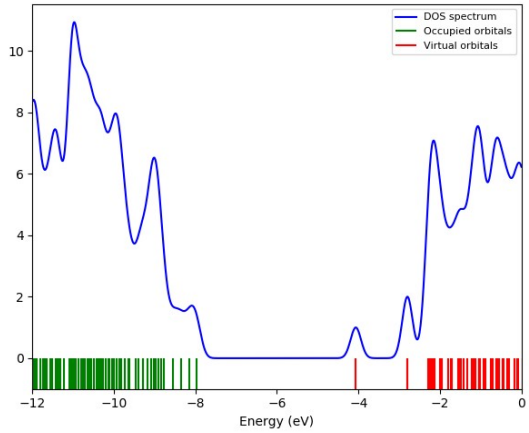
Table S3. HOMO, LUMO, band gap and adsorption energies (all in eV) of metal atoms and ions on BNNS and CP-BNNS complexes compared to bare and functionalized BNNS structures.

	HOMO	**LUMO**	E_g	E_d
BNNS	-6.45	-0.64	5.81	
Li@BNNS	-3.07	-0.66	2.41	-11.85
Li^+@BNNS	-7.98	-4.07	3.91	-49.97
Na@BNNS	-2.91	-0.66	2.25	-7.50
Na^+@BNNS	-7.96	-3.99	3.96	-32.35
PA-BNNS	-7.86	-4.28	3.58	536.18
Li@PA-BNNS	-7.42	-3.47	3.94	-33.30
Li^+@PA-BNNS	-9.75	-7.25	2.50	-6.97
Na@PA-BNNS	-7.90	-3.83	4.07	-23.16
Na^+@PA-BNNS	-9.91	-6.92	2.99	7.84
PP-BNNS	-6.66	-3.53	3.13	535.87
Li@PP-BNNS	-7.35	-3.62	3.73	-92.94
Li^+@PP-BNNS	-8.99	-6.04	2.95	-8.46
Na@PP-BNNS	-7.21	-3.49	3.72	-81.89
Na^+@PP-BNNS	-9.23	-5.17	4.06	-16.52
PPPh-BNNS	-7.81	-3.60	4.21	533.27
Li@PPPh-BNNS	-8.05	-4.28	3.78	-73.10
Li^+@PPPh-BNNS	-9.41	-6.18	3.23	-5.10
Na@PPPh-BNNS	-8.18	-4.12	4.06	-64.48
Na^+@PPPh-BNNS	-9.36	-6.31	3.05	6.49
PT-BNNS	-7.38	-4.05	3.33	539.47
Li@PT-BNNS	-7.90	-4.89	3.01	-94.64
Li^+@PT-BNNS	-9.22	-7.03	2.19	-5.48
Na@PT-BNNS	-7.77	-4.72	3.05	-82.41
Na^+@PT-BNNS	-10.07	-6.26	3.82	-9.62

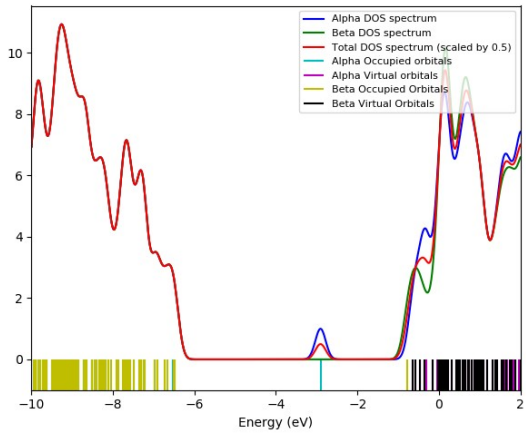
Li@BNNS



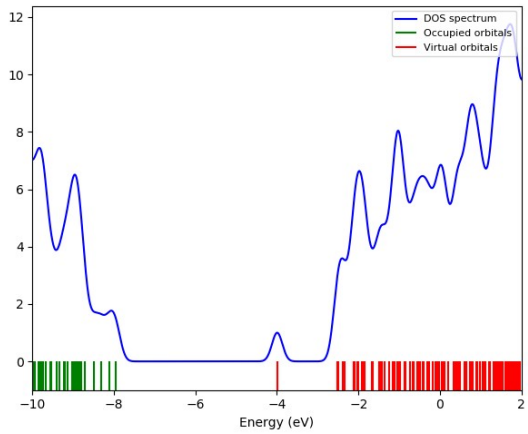
Li⁺@BNNS



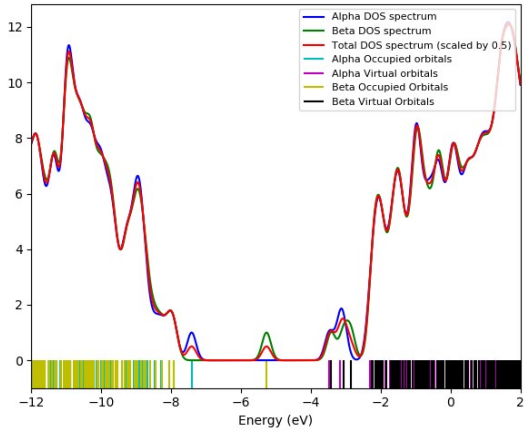
Na@BNNS



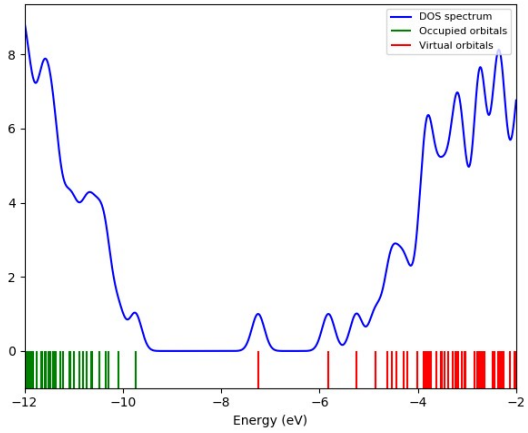
Na⁺@BNNS



Li@PA-BNNS

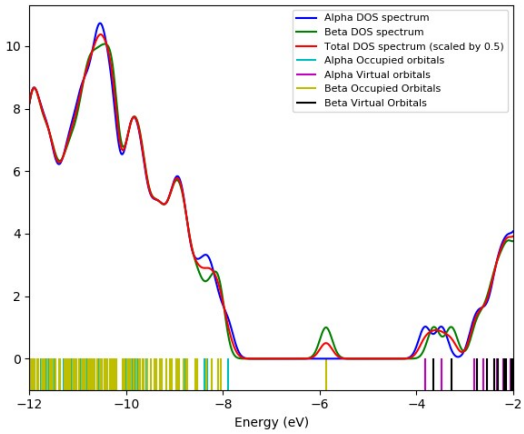


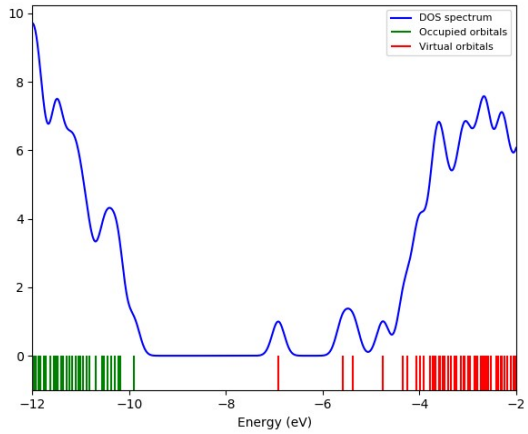
Li⁺@PA-BNNS



Na@PA-BNNS

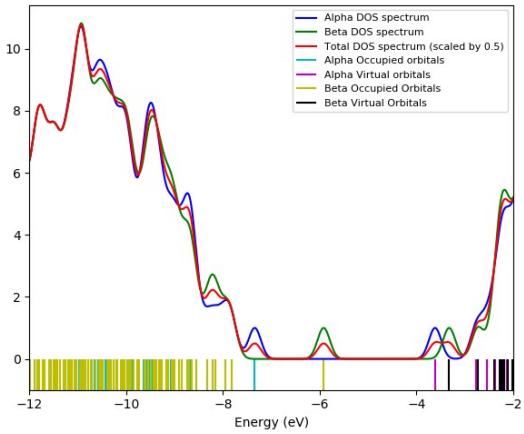
Na⁺@PA-BNNS

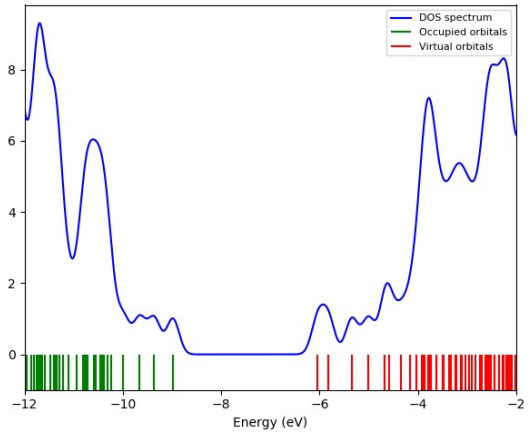




Li@PP-BNNS

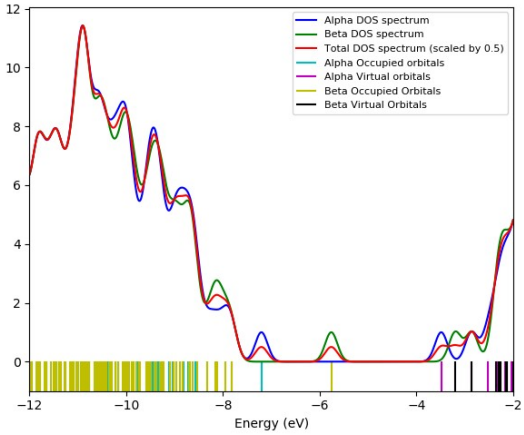
Li^{+}@PP-BNNS

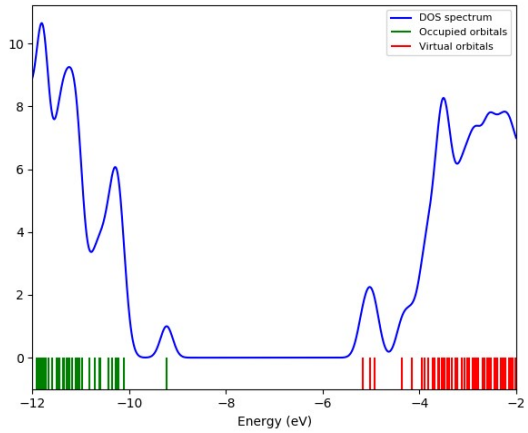




Na@PP-BNNS

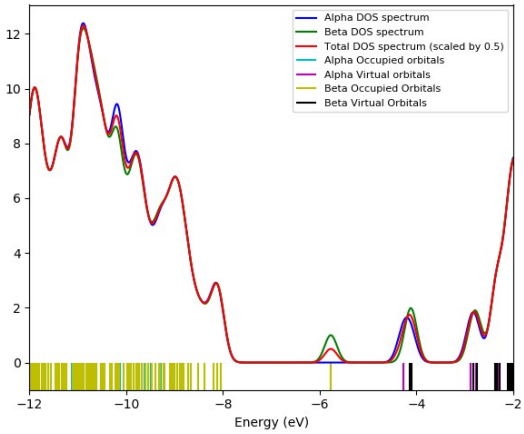
Na^{+}@PP-BNNS

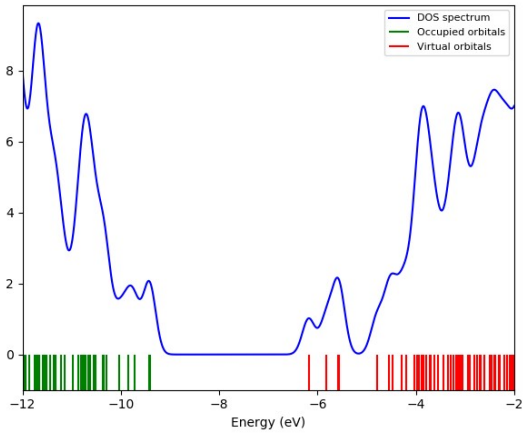




Li@PPPh-BNNS

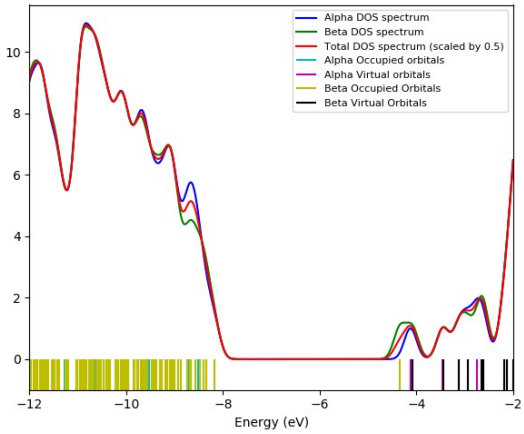
Li^{+}@PPPh-BNNS

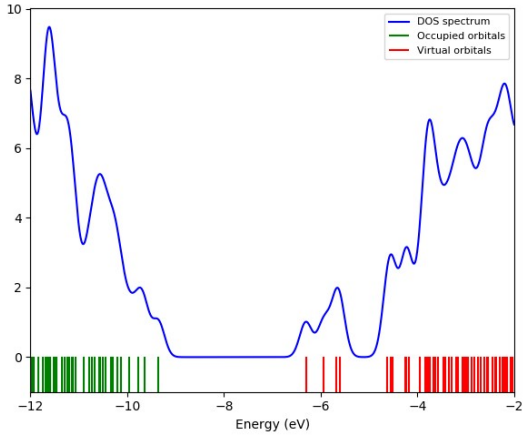




Na@PPPh-BNNS

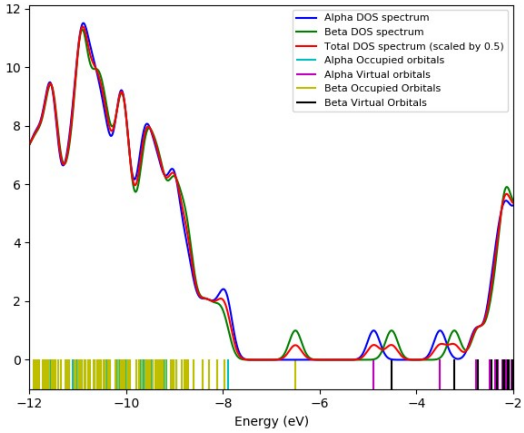
Na^{+}@PPPh-BNNS

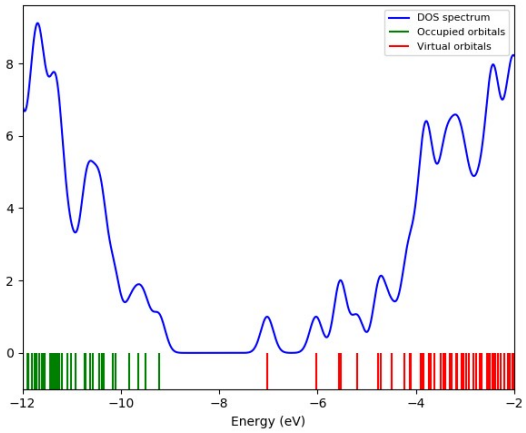




Li@PT-BNNS

Li^{+}@PT-BNNS





Na@PT-BNNS

Na^{+}@PT-BNNS

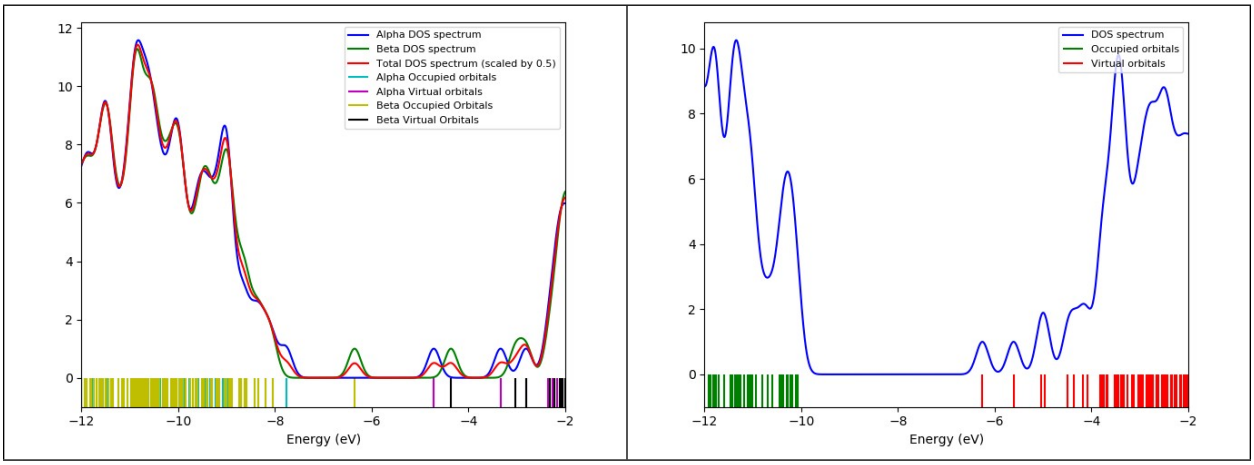
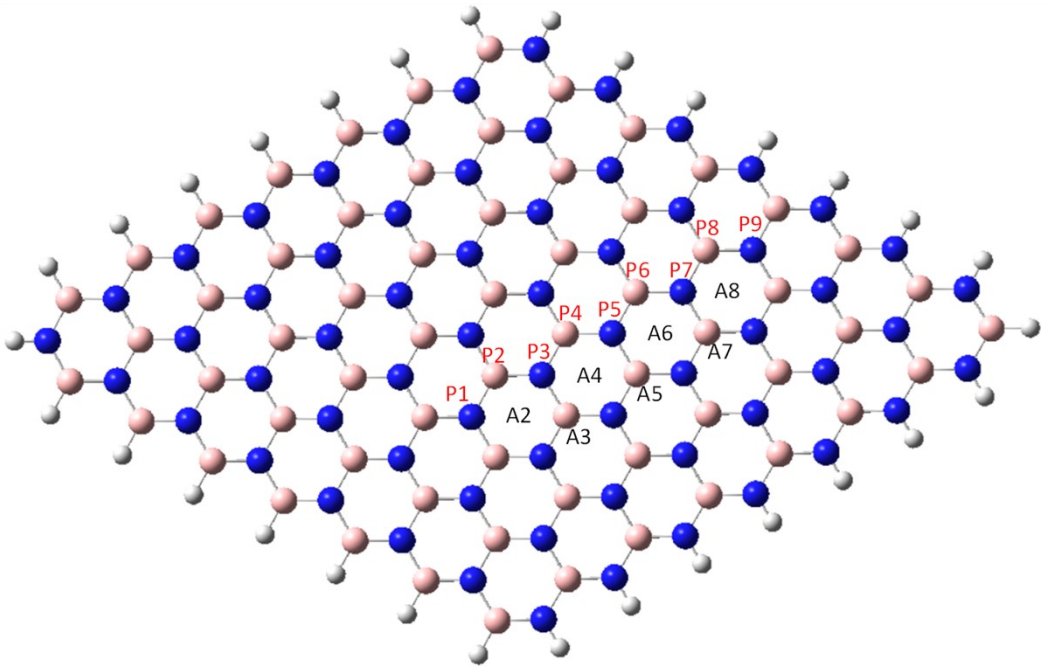


Figure S3. The density of States of the metal atoms and ions adsorbed onto the CP-BNNS.



Path 1 (via B-N bonds): P1-P2-P3-P4-P5-P6-P7-P8-P9

Path 2 (via ring-B): P1-A2-A3-A4-A5-A6-A7-A8-P9

Path 3 (via ring-N): P1-A2-P3-A4-P5-A6-P7-A8-P9

Figure S4. The pathway of ion diffusion on the sheets

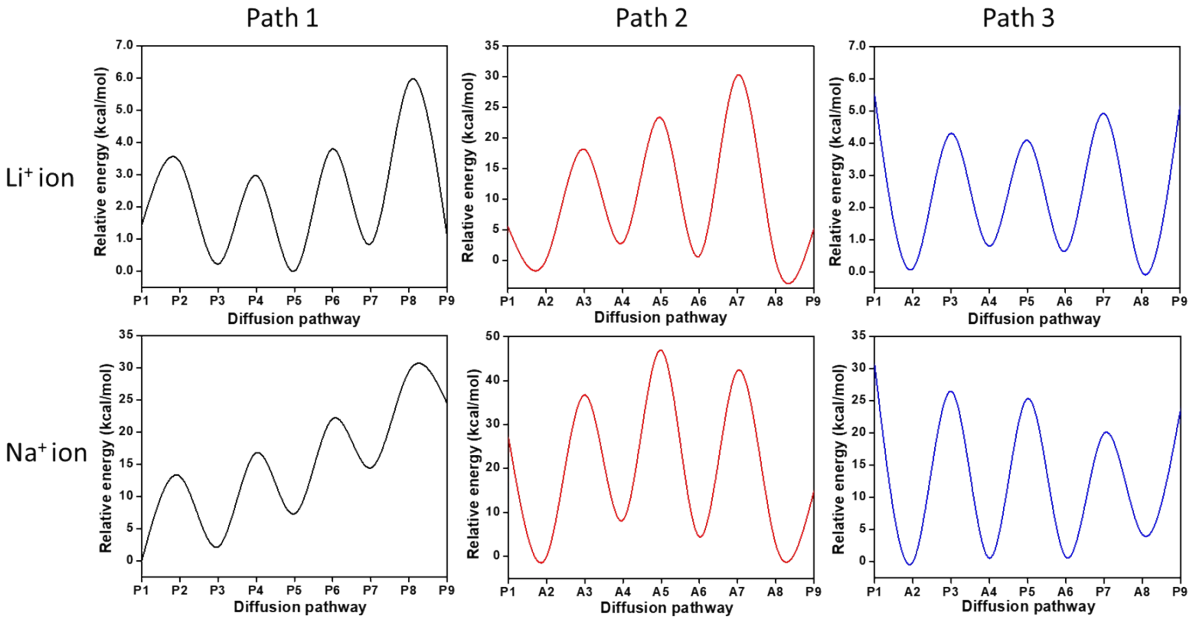


Figure S5. The diffusion profile of Li^+ and Na^+ ions via path 1, path 2 and path 3 on the pristine BNNS sheet

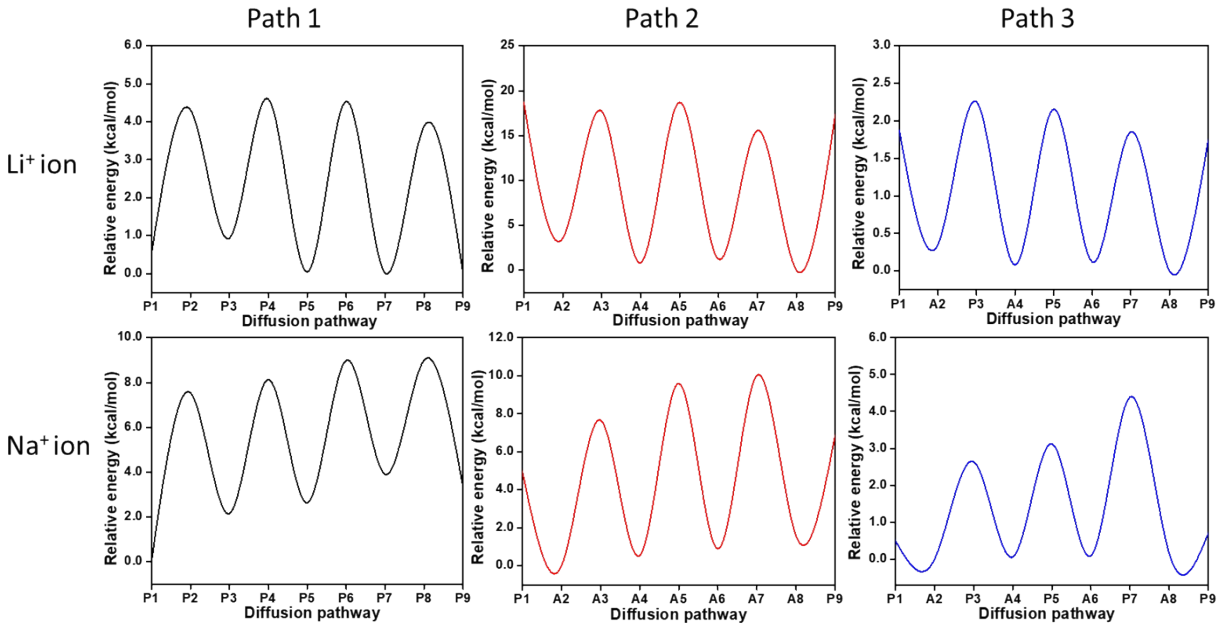


Figure S6. The diffusion profile of Li^+ and Na^+ ions via path 1, path 2 and path 3 on the PT functionalized BNNS sheet

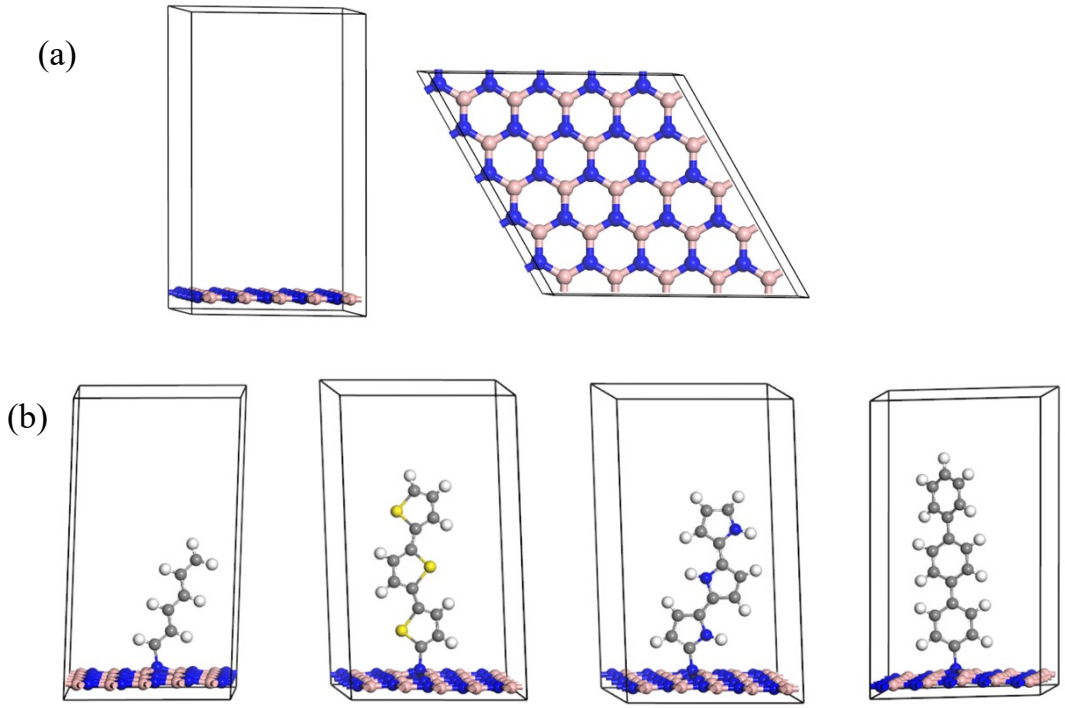


Figure S7 The geometrically optimized supercell with lattice dimensions of 12 × 12 × 20 Å of (a) BNNS, and the conducting polymer functionalized BNNS (b) from left to right: PA-BNNS, PT-BNNS, PP-BNNS and PPPh-BNNS

Table S4. The electronic properties of the pristine and the CP functionalized BNNS sheets

System	Cluster model			Periodic system		
	HOMO	**LUMO**	E_g	**HOMO**	**LUMO**	E_g
BNNS	-6.45	-0.64	5.81	-6.89	-1.02	5.87
PA-BNNS	-7.86	-4.28	3.58	-5.55	-3.14	2.41
Li@PA-BNNS	-7.42	-3.47	3.94	-5.75	-2.50	3.25
Li^+@PA-BNNS	-9.75	-7.25	2.50	-5.36	-3.19	2.18
Na@PA-BNNS	-7.90	-3.83	4.07	-7.01	-3.28	3.73
Na^+@PA-BNNS	-9.91	-6.92	2.99	-5.65	-3.25	2.39
PP-BNNS	-6.66	-3.53	3.13	-4.96	-2.69	2.27
Li@PP-BNNS	-7.35	-3.62	3.73	-4.88	-2.55	2.34
Li^+@PP-BNNS	-8.99	-6.04	2.95	-5.03	-2.92	2.11
Na@PP-BNNS	-7.21	-3.49	3.72	-4.87	-2.15	2.99
Na^+@PP-BNNS	-9.23	-5.17	4.06	-4.88	-1.11	3.77
PPPh-BNNS	-7.81	-3.60	4.21	-5.80	-2.41	3.38
Li@PPPh-BNNS	-8.05	-4.28	3.78	-5.64	-2.87	2.77
Li^+@PPPh-BNNS	-9.41	-6.18	3.23	-5.58	-2.89	2.69
Na@PPPh-BNNS	-8.18	-4.12	4.06	-5.81	-2.96	2.85
Na^+@PPPh-BNNS	-9.36	-6.31	3.05	-5.78	-3.20	2.58
PT-BNNS	-7.38	-4.05	3.33	-5.04	-2.56	2.48
Li@PT-BNNS	-7.90	-4.89	3.01	-5.14	-3.50	1.63
Li^+@PT-BNNS	-9.22	-7.03	2.19	-4.92	-3.44	1.48
Na@PT-BNNS	-7.77	-4.72	3.05	-5.05	-2.87	2.18
Na^+@PT-BNNS	-10.07	-6.26	3.82	-5.02	-1.76	3.27