Trends in Physisorption of Ionic Liquids on Boron-Nitride Sheet

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Table S1. Bond Critical Point Data (in au) obtained from QTAIM analysis for the H-bonds and other interactions in the ionic liquids based on $[Bmim]^+$, $[Bpy]^+$, and $[Btma]^+$ cations, paired with $[BF_4]^-$, $[PF_6]^-$, and $[Tf_2N]^-$ anions at the M06-2X/cc-pVDZ level of theory.

System	BCP	P(r)	Σρ(r)	$\nabla^2\rho(r)$	G(r)	V(r)	H(r)	$^aE_{(Y\ldots X)}$	$\Sigma E_{(Y\ldots X)}$
$[Bmim][BF_4]$	F20…H14	0.0171	0.1134	0.0572	0.0144	-0.0145	-0.0001	-4.56	-30.50
	F20…H13	0.0210		0.0772	0.0190	-0.0188	0.0002	-5.93	
	F22…H13	0.0168		0.0677	0.0160	-0.0150	0.0009	-4.73	
	F22…H18	0.0127		0.0538	0.0122	-0.0109	0.0012	-3.44	
	F22…H26	0.0068		0.0320	0.0066	-0.0053	0.0013	-1.66	
	F22…H16	0.0115		0.0503	0.0111	-0.0097	0.0014	-3.06	
	F21…H16	0.0113		0.0394	0.0095	-0.0092	0.0003	-2.89	
	F21…C2	0.0161		0.0634	0.0146	-0.0134	0.0012	-4.23	
$[Bmim][PF_6]$	F13…H18	0.0149	0.1145	0.0519	0.0129	-0.0128	0.0001	-4.02	-31.01
	F13…H20	0.0158		0.0594	0.0144	-0.0140	0.0004	-4.38	
	F14…H20	0.0183		0.0710	0.0171	-0.0166	0.0005	-5.22	
	F14…H24	0.0135		0.0585	0.0133	-0.0120	0.0013	-3.77	
	F14…H28	0.0076		0.0348	0.0074	-0.0061	0.0013	-1.92	
	F15…C2	0.0175		0.0689	0.0163	-0.0155	0.0008	-4.85	
	F15…H25	0.0135		0.0456	0.0114	-0.0115	-0.0001	-3.59	
	F16…H25	0.0066		0.0316	0.0065	-0.0052	0.00134	-1.64	
	F16…H29	0.0065		0.0285	0.0061	-0.0051	0.0010	-1.61	
$[Bmim][Tf_2N]$	O31…H11	0.0143	0.1163	0.0428	0.0107	-0.0108	-0.0001	-3.39	-25.70
	O31…C4	0.0075		0.0261	0.0055	-0.0045	0.0009	-1.42	
	N26…C2	0.0175		0.0614	0.0140	-0.0127	0.0013	-3.99	

	N26…H17	0.0105		0.0299	0.0070	-0.0066	0.0004	-2.09	
	O29…H6	0.0143		0.0510	0.0118	-0.0108	0.0009	-3.39	
	O29…H14	0.0125		0.0430	0.0101	-0.0095	0.0006	-2.98	
	O29…H20	0.0065		0.0242	0.0052	-0.0044	0.0008	-1.38	
	O30…H20	0.0054		0.0226	0.0045	-0.0034	0.0011	-1.10	
	O30…H23	0.0074		0.0277	0.0061	-0.0053	0.0008	-1.68	
	F40…H23	0.0026		0.0144	0.0026	-0.0016	0.0009	-0.52	
	F40…H17	0.0046		0.0206	0.0042	-0.0031	0.0009	-0.99	
	F38…H17	0.0050		0.0228	0.0046	-0.0035	0.0010	-1.11	
	F38…C5	0.0078		0.0312	0.0065	-0.0051	0.0013	-1.62	
[Bpy][BF_4]	C6 ...F27	0.0153	0.1018	0.0606	0.0138	-0.0124	0.0013	-3.91	-27.53
	H13...F29	0.0143		0.0574	0.0134	-0.0125	0.0009	-3.92	
	H17...F29	0.0105		0.0489	0.0105	-0.0088	0.0016	-2.78	
	H17...F27	0.0162		0.0529	0.0135	-0.0137	-0.0002	-4.31	
	H7...F28	0.0188		0.0767	0.0182	-0.0172	0.0009	-5.40	
	H7...F29	0.0184		0.0693	0.0169	-0.0165	0.0004	-5.18	
	H20...F29	0.0079		0.0353	0.0076	-0.0063	0.0012	-1.99	
[Bpy][PF_6]	N5...F31	0.0147	0.1087	0.0618	0.0139	-0.0123	0.0015	-3.88	-28.7
	C6...F26	0.0102		0.0438	0.0089	-0.0069	0.0020	-2.18	
	H7...F27	0.0169		0.0722	0.016	-0.0151	0.0014	-4.74	
	H17...F31	0.0149		0.0506	0.0127	-0.0129	-0.0001	-4.05	
	H17...F27	0.0106		0.0519	0.0109	-0.0089	0.0020	-2.80	
	H13...F27	0.0154		0.0676	0.0154	-0.0140	0.0014	-4.41	
	H17...F28	0.0093		0.0374	0.0085	-0.0077	0.0008	-2.42	
	H24...F28	0.0067		0.0297	0.0063	-0.0053	0.0010	-1.67	
	H20...F27	0.0095		0.0405	0.0090	-0.0079	0.0010	-2.50	
[Bpy][Tf_2N]	N5...N25	0.0133	0.0786	0.0481	0.0105	-0.0090	0.0014	-2.84	-16.93
	H16...N25	0.0099		0.0330	0.0072	-0.0063	0.0009	-1.97	
	H16...F35	0.0079		0.0373	0.0077	-0.0062	0.0015	-1.95	
	C6...O28	0.0116		0.0442	0.0094	-0.0077	0.0016	-2.44	
	C10...F37	0.0089		0.0393	0.0080	-0.0063	0.0017	-1.98	

	H17...O28	0.0102		0.0297	0.0073	-0.0071	0.0001	-2.25	
	C1...O30	0.0107		0.0398	0.0084	-0.0068	0.0015	-2.15	
	H22...F35	0.0058		0.0304	0.0058	-0.0041	0.0017	-1.31	
[Btma][BF_4]	F30…H4	0.0205	0.1123	0.0714	0.0178	-0.0179	-0.00001	-5.62	-30.38
	F30…H14	0.0121		0.0486	0.0112	-0.0104	0.0008	-3.27	
	F31…H14	0.0184		0.0619	0.0155	-0.0156	-0.0001	-4.90	
	F31…H22	0.0117		0.0406	0.0099	-0.0096	0.0002	-3.03	
	F30…H13	0.0181		0.0622	0.0157	-0.0159	-0.0001	-5.00	
	F28…H13	0.0160		0.0563	0.0139	-0.0139	0.0001	-4.36	
	F28…H19	0.0150		0.0587	0.0140	-0.0133	0.0006	-4.18	
[Btma][PF_6]	F29…H3	0.0147	0.1172	0.0501	0.0124	-0.0125	0.0001	-3.91	-31.89
	F29…H7	0.0171		0.0587	0.0148	-0.0149	-0.0001	-4.69	
	F31…H7	0.0158		0.0549	0.0137	-0.0137	-0.0001	-4.31	
	F31…H18	0.0126		0.0557	0.0126	-0.0113	0.0013	-3.56	
	F31…H21	0.0069		0.0330	0.0068	-0.0054	0.0014	-1.70	
	F31…H16	0.0156		0.0611	0.0147	-0.0141	0.0005	-4.43	
	F28…H16	0.0220		0.0763	0.0191	-0.0193	-0.0001	-6.04	
	F28…H3	0.0122		0.0452	0.0108	-0.0104	0.0004	-3.25	
[Btma][Tf_2N]	O32…H3	0.0157	0.1307	0.0520	0.0126	-0.0122	0.0003	-3.83	-30.23
	O32…H16	0.0121		0.0362	0.0090	-0.0090	-0.0001	-2.85	
	F39…H16	0.0080		0.0316	0.0071	-0.0064	0.0007	-2.02	
	F39…H21	0.0057		0.0253	0.0052	-0.0042	0.0010	-1.33	
	O32…H7	0.0142		0.0418	0.0106	-0.0108	-0.0001	-3.39	
	N27…H7	0.0127		0.0403	0.0094	-0.0087	0.0006	-2.76	
	N27…H16	0.0144		0.0457	0.0108	-0.0102	0.0006	-3.20	
	N27…H18	0.0098		0.0354	0.0077	-0.0066	0.0011	-2.08	
	N27…H21	0.0078		0.0249	0.0056	-0.0050	0.0006	-1.57	
	O30…H25	0.0112		0.0384	0.0091	-0.0086	0.0004	-2.71	
	O30…H18	0.0116		0.0356	0.0088	-0.0087	0.0001	-2.74	
	F37…H9	0.0069		0.0318	0.0067	-0.0056	0.0011	-1.75	

[a] X = N, O, F and Y = H, C, N, $E_{Y\ldots X}$ (in kcal/mol)

Table S2. Bond Critical Point Data (in au) obtained from QTAIM analysis for the H-bonds and other interactions in the ionic liquids adsorbed on *h*-BN surface at the M06-2X/cc-pVDZ level of theory

System	BCPs	ρ(r)	∑ρ(r)	$\nabla^2\rho(r)$	G(r)	V(r)	H(r)	$^aE_{(Y...X)}$	$\Sigma E_{(Y...X)}$
BN[Bmim][BF_4]	H85...F92	0.0264	0.0937	0.0995	0.0238	-0.0228	0.0010	-7.18	-24.60
	H85...F94	0.0159		0.0613	0.0147	-0.0140	0.0006	-4.41	
	H90...F94	0.0138		0.0569	0.0132	-0.0122	0.0009	-3.84	
	H88...F94	0.0113		0.0501	0.0110	-0.0095	0.0014	-2.99	
	H88...F93	0.0115		0.0390	0.0095	-0.0093	0.0002	-2.92	
	F94...H98	0.0076		0.0343	0.0072	-0.0059	0.0013	-1.87	
	H86...F92	0.0041		0.0201	0.0038	-0.0026	0.0011	-0.83	
	F93...H102	0.0028		0.0148	0.0027	-0.0017	0.0009	-0.53	
BN[Bmim][PF_6]	F15...H25	0.0056	0.0971	0.0257	0.0053	-0.0041	0.0011	-1.30	-26.0432
	C2...F15	0.0158		0.0628	0.0146	-0.0134	0.0011	-4.23	
	F14...H25	0.0105		0.0472	0.0103	-0.0088	0.0014	-2.78	
	F14...H24	0.0127		0.0559	0.0126	-0.0112	0.0013	-3.54	
	F13...H20	0.0186		0.0674	0.0167	-0.0165	0.0001	-5.20	
	F13...H18	0.0127		0.0450	0.0109	-0.0107	0.0002	-3.35	
	F14...H20	0.0151		0.0618	0.0144	-0.0134	0.0010	-4.20	
	F14...H28	0.0058		0.0288	0.0058	-0.0045	0.0013	-1.41	
BN[Bmim][Tf_2N]	C74...N98	0.0168	0.1124	0.0584	0.0132	-0.0119	0.0013	-3.74	-25.09
	C76...O103	0.0074		0.0258	0.0054	-0.0044	0.0009	-1.39	
	C77...F110	0.0087		0.0344	0.0072	-0.0059	0.0013	-1.86	
	H78...O101	0.0142		0.0516	0.0118	-0.0107	0.0010	-3.37	
	H89...N98	0.0100		0.0288	0.0067	-0.0062	0.0004	-1.95	
	H89...F112	0.0070		0.0281	0.0062	-0.0053	0.0008	-1.68	
	H86...O101	0.0119		0.0451	0.0102	-0.0091	0.0010	-2.86	
	H95...F112	0.0036		0.0191	0.0036	-0.0025	0.0011	-0.79	
	H95...O102	0.0085		0.0276	0.006	-0.0061	0.0004	-1.91	
	H92...O101	0.0081		0.0299	0.0066	-0.0058	0.0008	-1.83	
	H83...O103	0.0136		0.0410	0.0102	-0.0103	0.0000	-3.23	
	H82...F108	0.0021		0.0126	0.0022	-0.0013	0.0009	-0.42	
BN[BPy][BF_4]	H7...F29	0.0169	0.0915	0.0609	0.0149	-0.0145	0.0003	-4.57	-24.33
	H13...F29	0.0155		0.0599	0.0143	-0.0138	0.0005	-4.33	
	H17...F27	0.0124		0.0413	0.0102	-0.0101	0.0001	-3.17	
	H7...F28	0.0228		0.0830	0.0203	-0.0200	0.0003	-6.27	
	H17...F29	0.0104		0.0483	0.0103	-0.0087	0.0016	-2.73	
	H24...F27	0.0044		0.0209	0.0041	-0.0030	0.0010	-0.95	
	H20...F29	0.0089		0.0382	0.0084	-0.0072	0.0011	-2.27	
BN[BPy][PF_6]	H85...F99	0.0138	0.1034	0.0546	0.0129	-0.0122	0.0006	-3.85	-27.74
	H92...F99	0.0088		0.0371	0.0082	-0.0072	0.0010	-2.25	
	H79...F103	0.0164		0.0608	0.0149	-0.0146	0.0002	-4.59	

	H89...F99	0.0077		0.0392	0.0079	-0.0060	0.0018	-1.89	
	H96...F100	0.0068		0.0297	0.0064	-0.0053	0.0010	-1.68	
	H79...F98	0.0131		0.0490	0.0117	-0.0111	0.0005	-3.51	
	H79...F99	0.0190		0.0668	0.0166	-0.0165	0.0001	-5.20	
	H89...F103	0.0174		0.0575	0.0147	-0.0150	-0.0003	-4.73	
BN[BPy][Tf_2N]	H88...F107	0.0119	0.077	0.0465	0.0109	-0.0102	0.0007	-3.20	-16.00
	C82...F109	0.0076		0.0368	0.0072	-0.0057	0.0015	-1.79	
	C78...N97	0.0101		0.0354	0.0077	-0.0065	0.0011	-2.03	
	C78...O100	0.0085		0.0334	0.0068	-0.0053	0.0015	-1.66	
	H89...O100	0.0146		0.0406	0.0104	-0.0108	-0.0003	-3.38	
	C75...O102	0.0121		0.0441	0.0095	-0.0079	0.0015	-2.47	
	H94...F107	0.0062		0.0274	0.0057	-0.0047	0.0010	-1.47	
BN[Btma][BF_4]	H86...F102	0.0158	0.1087	0.0542	0.0136	-0.0137	0.0000	-4.30	-29.03
	H86...F103	0.0129		0.0495	0.0117	-0.0110	0.0006	-3.48	
	H94...F103	0.0125		0.0493	0.0115	-0.0108	0.0007	-3.40	
	H85...F102	0.0137		0.0500	0.0121	-0.0118	0.0003	-3.70	
	H85...F100	0.0194		0.0666	0.0167	-0.0168	0.0000	-5.28	
	H91...F100	0.0086		0.0334	0.0075	-0.0067	0.0007	-2.12	
	H91...F103	0.0089		0.0427	0.0089	-0.0071	0.0017	-2.24	
	H76...F102	0.0164		0.0582	0.0144	-0.0142	0.0001	-4.48	
BN[Btma][PF_6]	H87...F99	0.0192	0.0982	0.0653	0.0165	-0.0167	-0.0001	-5.24	-26.54
	H74...F99	0.0155		0.0540	0.0134	-0.0134	0.0001	-4.22	
	H74...F100	0.0092		0.0363	0.0083	-0.0075	0.0007	-2.36	
	H78...F100	0.0151		0.0517	0.0129	-0.0129	0.0000	-4.05	
	H87...F102	0.0136		0.0535	0.0127	-0.0120	0.0006	-3.78	
	H78...F102	0.0135		0.0480	0.0117	-0.0115	0.0002	-3.62	
	H89...F102	0.0118		0.0497	0.0114	-0.0104	0.0010	-3.26	
BN[Btma][Tf_2N]	H78...O103	0.0139	0.116	0.0411	0.0104	-0.0105	-0.0001	-3.30	-26.37
	H78...N98	0.0113		0.0367	0.0083	-0.0075	0.0008	-2.36	
	H87...N98	0.0138		0.0445	0.0104	-0.0097	0.0006	-3.06	
	H89...N98	0.0102		0.0372	0.0081	-0.0069	0.0011	-2.17	
	H89...O101	0.0128		0.0379	0.0096	-0.0097	-0.0001	-3.04	
	H87...O103	0.0112		0.0340	0.0084	-0.0083	0.0001	-2.62	
	H78...F108	0.0077		0.0385	0.0079	-0.0062	0.0017	-1.95	
	H92...F110	0.0038		0.0184	0.0036	-0.0026	0.0010	-0.81	
	H92...N98	0.0084		0.0264	0.0060	-0.0054	0.0006	-1.69	
	H96...O101	0.0097		0.0316	0.0075	-0.0071	0.0003	-2.25	
	H74...O103	0.0128		0.0421	0.0101	-0.0097	0.0003	-3.07	

[a] X = N, O, F and Y = H, C, $E_{Y...X}$ (in kcal/mol)

Table S3. Bond Critical Point Data (in au) obtained from QTAIM analysis for the interactions between $[Bmim]^+$, $[Bpy]^+$, and $[Btma]^+$ cations of ILs and *h*-BN surface at the M06-2X/cc-pVDZ level of theory

System	BCPs between cation & *h*-BN	ρ(r)	∑ ρ(r)	$\nabla^2\rho(r)$	G(r)	V(r)	H(r)	$^aE_{(Y\ldots X)}$	$\sum E_{(Y\ldots X)}$
BN[bmim][BF_4]	N43…H84	0.0090	0.0535	0.0310	0.0064	-0.0050	0.0013	-1.59	-9.59
	N18…H90	0.0085		0.0279	0.0060	-0.0051	0.0009	-1.61	
	N7…H90	0.0078		0.0264	0.0056	-0.0047	0.0009	-1.49	
	N19…H90	0.0072		0.0274	0.0055	-0.0041	0.0013	-1.31	
	N31…N73	0.0072		0.0228	0.0048	-0.0040	0.0008	-1.27	
	N31…N75	0.0070		0.0220	0.0047	-0.0040	0.0007	-1.27	
	N31…C77	0.0068		0.0195	0.0041	-0.0033	0.0007	-1.05	
BN[bmim][PF_6]	H25...N50	0.0034	0.0476	0.0119	0.0022	-0.0015	0.0007	-0.49	-8.34
	H26...N59	0.0049		0.0173	0.0034	-0.0025	0.0009	-0.79	
	C4...N71	0.0086		0.0311	0.0061	-0.0044	0.0016	-1.40	
	H21...N81	0.0094		0.0283	0.0063	-0.0056	0.0006	-1.78	
	H32...N74	0.0067		0.0218	0.0046	-0.0038	0.0008	-1.19	
	H29...N39	0.0073		0.0235	0.0050	-0.0041	0.0008	-1.30	
	H31...B37	0.0073		0.0258	0.0054	-0.004	0.0010	-1.39	
BN[bmim][Tf_2N]	N7...H95	0.0072	0.0072	0.0255	0.0050	-0.0037	0.0013	-1.17	-1.17
BN[Bpy][BF_4]	H13...N59	0.0084	0.0436	0.0272	0.0059	-0.005	0.0008	-1.57	-7.35
	C3...N44	0.0067		0.0197	0.0040	-0.0032	0.0008	-1.01	
	C3...N36	0.0068		0.0198	0.0040	-0.0031	0.0008	-1.00	
	C8...N47	0.0074		0.0223	0.0046	-0.0036	0.0009	-1.15	
	H13...N56	0.0066		0.0251	0.0049	-0.0036	0.0013	-1.15	
	H13...N68	0.0077		0.0262	0.0056	-0.0046	0.0009	-1.47	
BN[Bpy][PF_6]	N18...H85	0.0099	0.0381	0.0312	0.0069	-0.0061	0.0008	-1.93	-6.66
	N4...C75	0.0066		0.0198	0.0040	-0.0032	0.0008	-1.01	
	N7...N77	0.0071		0.0230	0.0050	-0.0044	0.0006	-1.38	
	N15...H86	0.0070		0.0244	0.0048	-0.0036	0.0012	-1.13	
	N7 ...C80	0.0075		0.0231	0.0048	-0.0038	0.0009	-1.21	
BN[Bpy][Tf_2N]	N27...H86	0.0054	0.0488	0.0177	0.0036	-0.0028	0.0007	-0.89	-8.84
	N15...H74	0.0065		0.0221	0.0046	-0.0038	0.0008	-1.19	
	N27...H74	0.0065		0.0218	0.0046	-0.0037	0.0008	-1.18	
	N18...H74	0.0068		0.0220	0.0047	-0.0039	0.0007	-1.23	
	N31...H88	0.0055		0.0180	0.0037	-0.0029	0.0007	-0.92	
	N42...H91	0.0096		0.0294	0.0065	-0.0057	0.0007	-1.81	
	N43...H94	0.0085		0.0283	0.0061	-0.0051	0.0009	-1.62	
BN[Btma][BF_4]	N18...H94	0.0085	0.0476	0.0273	0.0059	-0.0051	0.0008	-1.61	-9.01
	N31 - H86	0.0073		0.0223	0.0048	-0.0040	0.0007	-1.27	
	N22...H75	0.0087		0.0290	0.0064	-0.0055	0.0008	-1.74	
	N34...H75	0.0088		0.0312	0.0066	-0.0055	0.0011	-1.72	

	N19...H88	0.0062		0.0214	0.0044	-0.0035	0.0009	-1.10	
	N7...H94	0.0081		0.0286	0.0060	-0.0050	0.0010	-1.57	
BN[Btma][PF_6]	N30...H75	0.0086	0.0459	0.0289	0.0062	-0.0052	0.0010	-1.63	-8.46
	N27...H75	0.0081		0.0285	0.0060	-0.0050	0.0010	-1.57	
	N39...H75	0.0079		0.0259	0.0056	-0.0047	0.0008	-1.50	
	N42...H85	0.0076		0.0229	0.0050	-0.0043	0.0006	-1.37	
	N43...H93	0.0071		0.0252	0.0051	-0.0039	0.0011	-1.24	
	N34...H92	0.0066		0.0224	0.0046	-0.0036	0.0009	-1.15	
BN[Btma][Tf_2N]	N18...H79	0.0078	0.0181	0.0233	0.0051	-0.0044	0.0006	-1.39	-3.36
	N19...H76	0.0103		0.0309	0.0070	-0.0062	0.0007	-1.97	

[a] X , Y = H, C, B, N, $E_{Y...X}$ (in kcal/mol)

Table S4. Bond Critical Point Data (in au) obtained from QTAIM analysis for the interactions between $[BF_4]^-$, $[PF_6]^-$, and $[Tf_2N]^-$ anions of ILs and *h*-BN surface at the M06-2X/cc-pVDZ level of theory

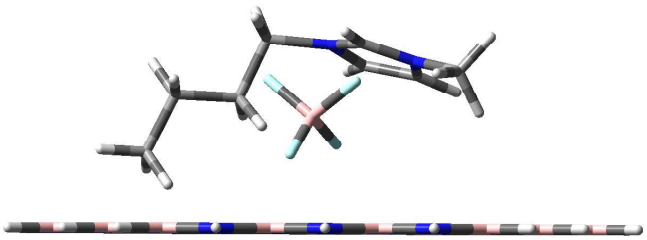
System	BCPs between anion & *h*-BN	ρ(r)	∑ρ(r)	$\nabla^2\rho(r)$	G(r)	V(r)	H(r)	$^aE_{(Y\ldots X)}$	$\Sigma E_{(Y\ldots X)}$
BN[bmim][BF_4]	N27…F94	0.0100	0.0771	0.0416	0.0089	-0.0075	0.0014	-2.37	-17.92
	N18…F94	0.0097		0.0399	0.0086	-0.0074	0.0012	-2.32	
	N27…F95	0.0088		0.0379	0.0079	-0.0064	0.0015	-2.02	
	N27…F92	0.0087		0.0371	0.0078	-0.0063	0.0014	-1.98	
	N15…F94	0.0085		0.0367	0.0077	-0.0063	0.0014	-2.00	
	N14…F95	0.0082		0.0346	0.0073	-0.0061	0.0012	-1.91	
	N39…F92	0.0081		0.0345	0.0073	-0.0059	0.0013	-1.88	
	N26…F95	0.0075		0.0327	0.0068	-0.0054	0.0013	-1.71	
	N30…F92	0.0076		0.0322	0.0067	-0.0055	0.0012	-1.73	
BN[bmim][PF_6]	F15...B64	0.0111	0.0347	0.0426	0.0101	-0.0095	0.0005	-3.00	-9.48
	F16...N51	0.0112		0.0424	0.0100	-0.0095	0.0005	-2.98	
	F12...B65	0.0124		0.0469	0.0114	-0.0111	0.0002	-3.50	
BN[bmim][Tf_2N]	N19...O102	0.0108	0.0537	0.0431	0.0093	-0.0078	0.0014	-2.45	-12.67
	N18...F112	0.0084		0.0338	0.0074	-0.0064	0.0010	-2.02	
	N30...F111	0.0074		0.0312	0.0066	-0.0055	0.0011	-1.73	
	N43...O104	0.0120		0.0437	0.0100	-0.0091	0.0009	-2.86	
	B24...F109	0.0072		0.0307	0.0066	-0.0055	0.0010	-1.74	
	N34...F107	0.0079		0.0337	0.0072	-0.0059	0.0012	-1.87	
BN[Bpy][BF_4]	F29...N59	0.0088	0.0690	0.0376	0.0080	-0.0066	0.0013	-2.07	-15.96
	F29...N72	0.0094		0.0401	0.0085	-0.0070	0.0015	-2.20	
	F29...N71	0.0094		0.0394	0.0084	-0.0070	0.0014	-2.21	
	F28...N72	0.0091		0.0384	0.0081	-0.0066	0.0014	-2.09	
	F28...N63	0.0080		0.0341	0.0072	-0.0059	0.0012	-1.87	
	F26...N72	0.0085		0.0368	0.0076	-0.0061	0.0015	-1.92	
	F26...N75	0.0077		0.033	0.0069	-0.0056	0.0013	-1.75	
	F26...N81	0.0081		0.0343	0.0072	-0.0059	0.0013	-1.85	
BN[Bpy][PF_6]	N31...F99	0.0075	0.0341	0.0318	0.0066	-0.0053	0.0012	-1.68	-8.06
	N43...F101	0.0108		0.0464	0.0100	-0.0085	0.0015	-2.68	
	N31...F98	0.0089		0.0364	0.0079	-0.0067	0.0011	-2.12	
	N30...F99	0.0069		0.0303	0.0063	-0.0050	0.0012	-1.58	
BN[Bpy][Tf_2N]	N22...F107	0.0079	0.0356	0.0330	0.0073	-0.0063	0.0009	-1.98	-9.64
	N7...O102	0.0150		0.0517	0.0124	-0.0120	0.0004	-3.77	
	N8...F110	0.0022		0.0117	0.0065	-0.0047	0.0018	-1.47	
	N11...O103	0.0105		0.0357	0.0083	-0.0077	0.0006	-2.42	
BN[Btma][BF_4]	B29...F103	0.0128	0.0346	0.0460	0.0113	-0.0111	0.0001	-3.50	-9.23
	B32...F102	0.0102		0.0382	0.0089	-0.0083	0.0006	-2.62	
	B41...F101	0.0116		0.0426	0.0102	-0.0099	0.0003	-3.11	

BN[Btma][PF_6]	B20...F99	0.0155	0.0351	0.0562	0.0144	-0.0147	-0.0003	-4.63	-9.72
	N19...F104	0.0086		0.0341	0.0076	-0.0067	0.0008	-2.11	
	B21...F103	0.0110		0.0423	0.0100	-0.0095	0.0005	-2.98	
BN[Btma][Tf_2N]	N34...O103	0.0104	0.0420	0.0346	0.0082	-0.0077	0.0004	-2.44	-9.89
	N52...O104	0.0117		0.0420	0.0095	-0.0086	0.0009	-2.71	
	N42...F108	0.0103		0.0402	0.0091	-0.0082	0.0009	-2.58	
	N42…F107	0.0079		0.0328	0.0072	-0.0061	0.0010	-1.93	
	B48...F111	0.0017		0.0087	0.0014	-0.0007	0.0007	-0.23	

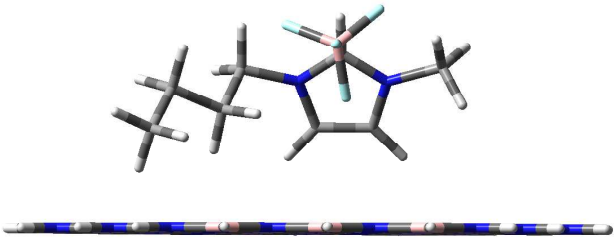
[a] X , Y = N, O, B, F, $E_{Y...X}$ (in kcal/mol)

Table S5. Changes in the binding energy (ΔE_b in kcal/mol), enthalpy (ΔH_{ads} in kcal/mol), free energy (ΔG_{ads} in kcal/mol), entropy (ΔS_{ads} in cal/mol.K), translational entropy (ΔS_t in cal/mol.K), rotational entropy (ΔS_r in cal/mol.K), and vibrational entropy (ΔS_v in cal/mol.K) of ILs upon adsorption on the *h*-BN surface

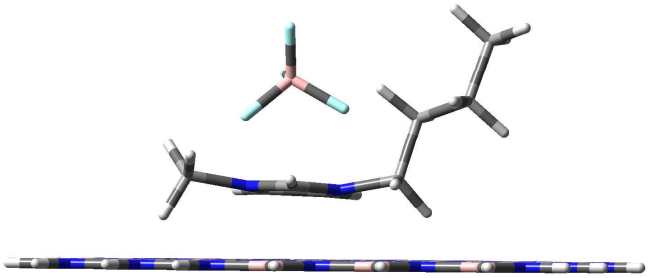
Structure	ΔE_b	ΔH_{ads}	ΔG_{ads}	ΔS_{ads}	ΔS_t	ΔS_r	ΔS_v
[Bmim][BF_4]	-21.21	-21.80	-6.743	-50.49	-41.309	-31.612	22.426
[Bmim][PF_6]	-21.26	-21.85	-7.33	-48.71	-41.807	-32.192	25.285
[Bmim][Tf_2N]	-17.85	-18.44	-4.47	-46.85	-42.581	-33.418	29.144
[Bpy][BF_4]	-23.03	-23.62	-8.16	-51.86	-41.279	-31.609	21.029
[Bpy][PF_6]	-21.72	-22.31	-8.66	-45.78	-41.785	-32.023	28.03
[Bpy][Tf_2N]	-18.86	-19.46	-3.93	-52.04	-42.567	-33.444	23.966
[Btma][BF_4]	-20.15	-20.74	-7.13	-45.65	-41.066	-31.166	26.577
[Btma][PF_6]	-19.81	-20.40	-7.61	-42.89	-41.627	-31.972	30.712
[Btma][Tf_2N]	-18.45	-19.05	-3.98	-50.52	-42.475	-33.25	25.203



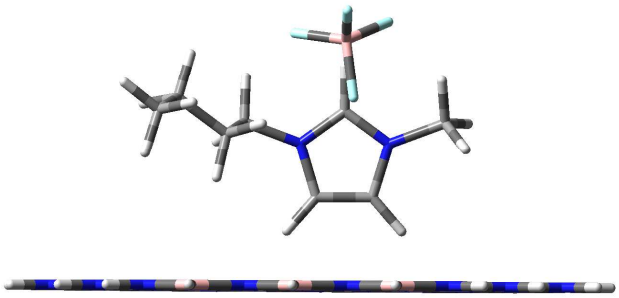
BN[Bmim][BF_4]1



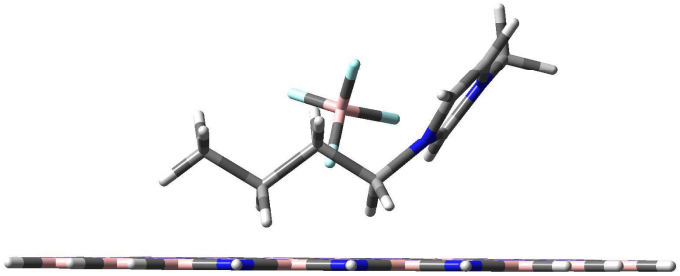
BN[Bmim][BF_4]2



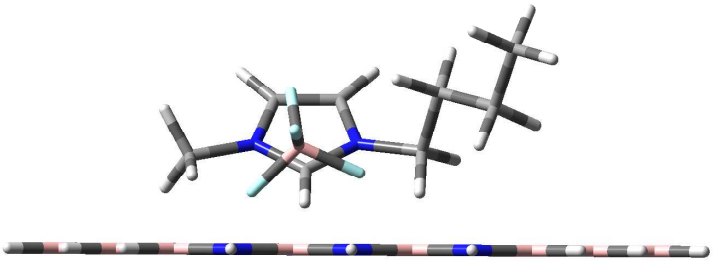
BN[Bmim][BF_4]3



BN[Bmim][BF_4]4



BN[Bmim][BF_4]5



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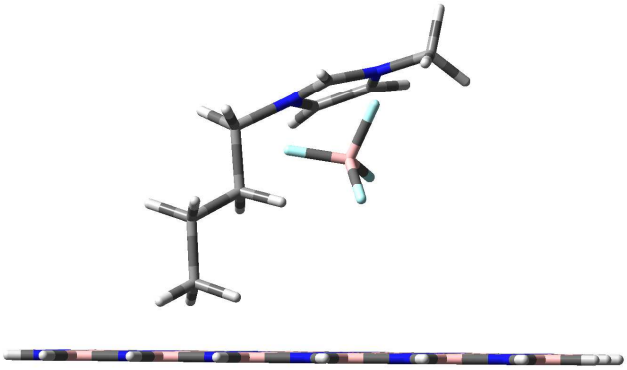
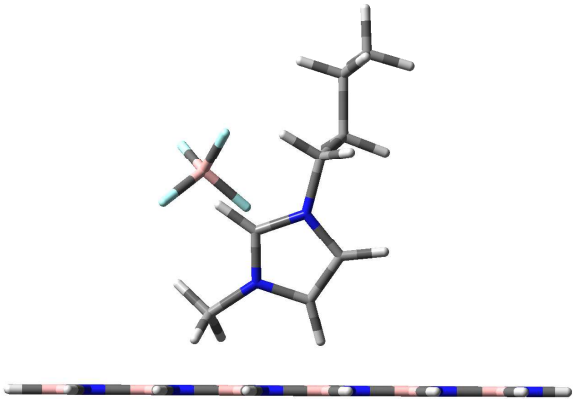
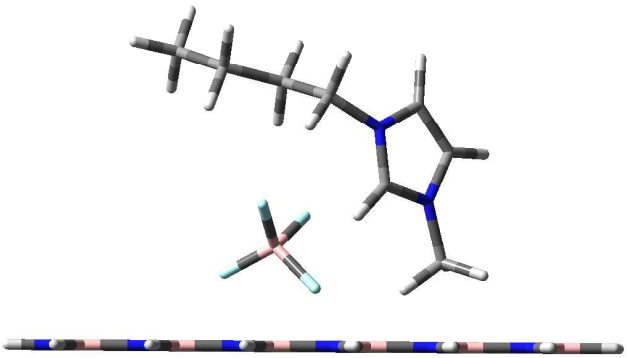


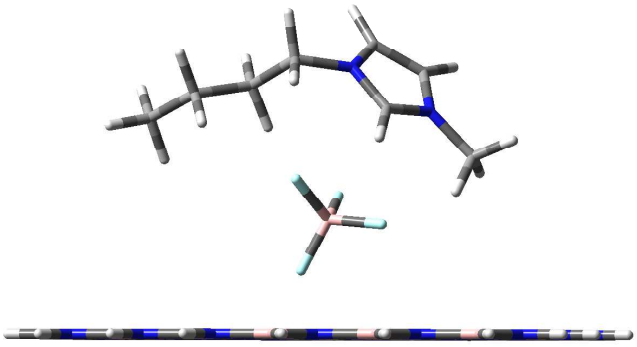
BN[Bmim][BF_4]7



BN[Bmim][BF_4]8

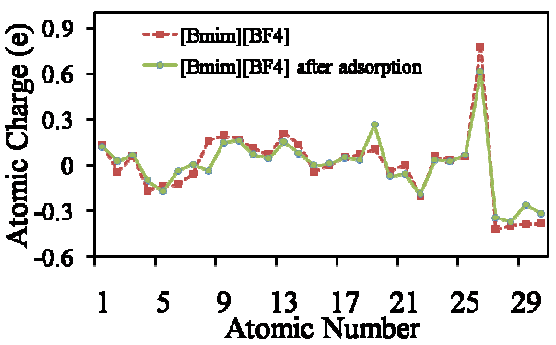


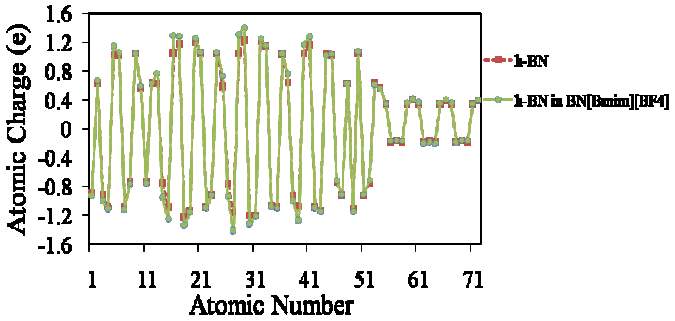
BN[Bmim][BF_4]9

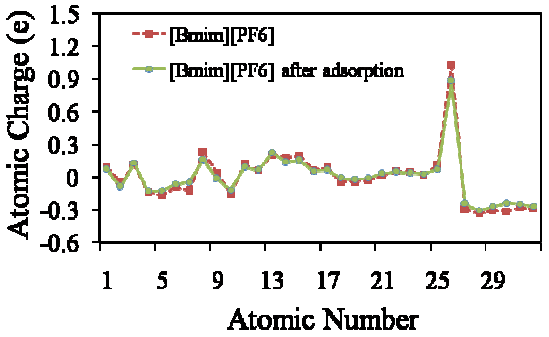


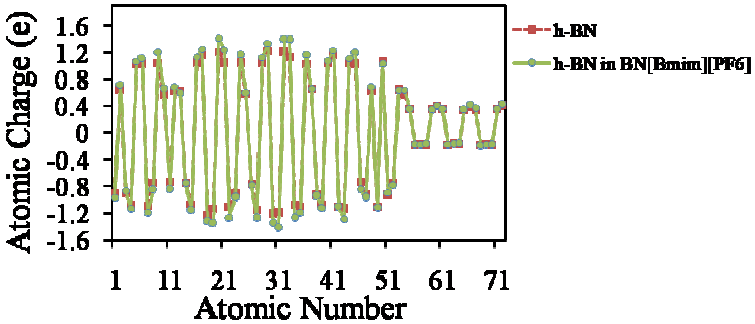
BN[Bmim][BF_4]10

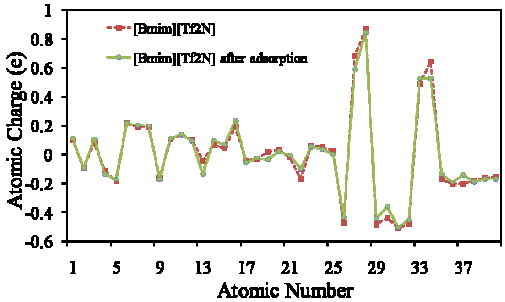
Figure S1. The initial structures for adsorption of [Bmim][BF_4] ionic liquid on the *h*-BN surface

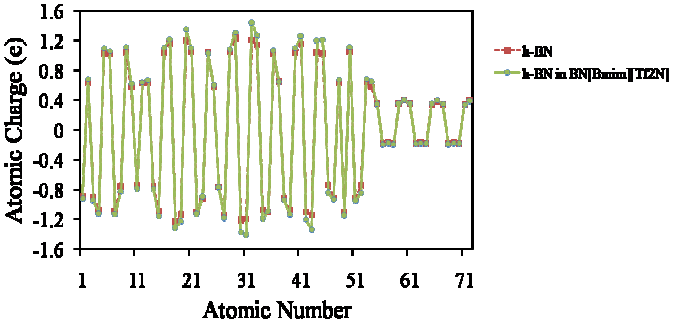

[Bmim][BF4]
[Bmim][BF4] after adsorption
Atomic Charge (e)
Atomic Number

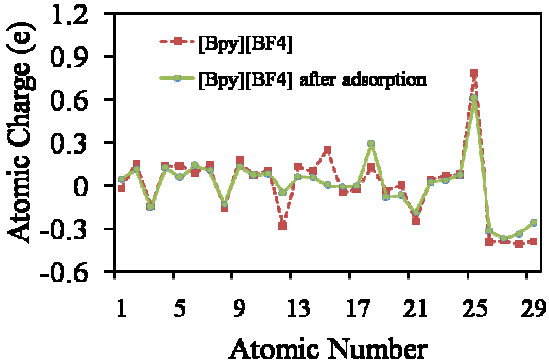

h-BN
h-BN in BN[Bmim][BF4]
Atomic Charge (e)
Atomic Number

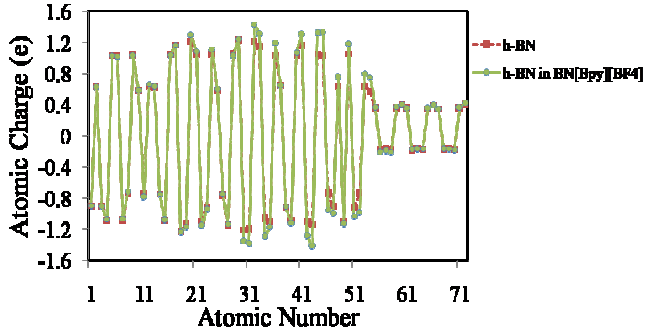

[Bmim][PF6]
[Bmim][PF6] after adsorption
Atomic Charge (e)
Atomic Number

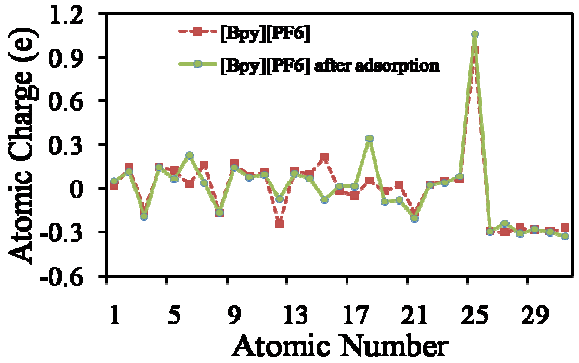

h-BN
h-BN in BN[Bmim][PF6]
Atomic Charge (e)
Atomic Number

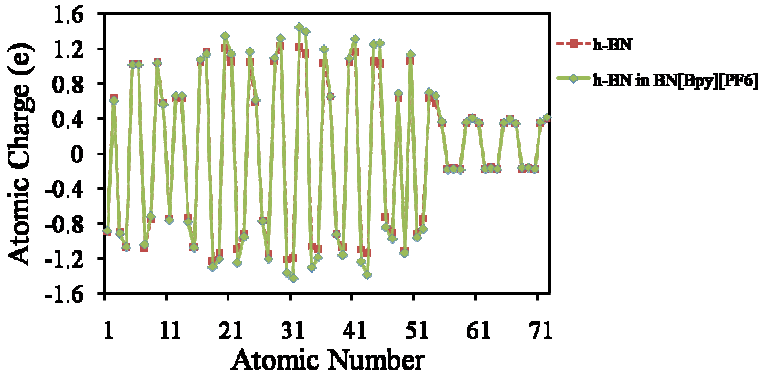

[Bmim][Tf2N]
[Bmim][Tf2N] after adsorption
Atomic Charge (e)
Atomic Number

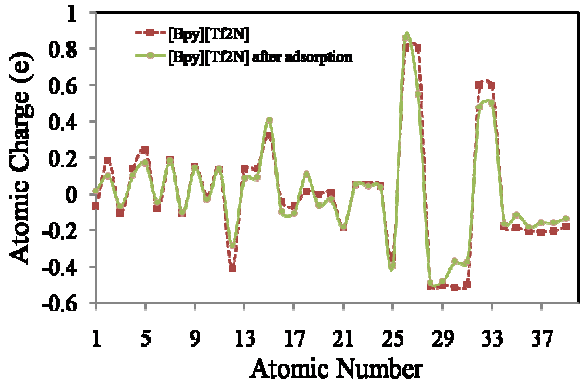

h-BN
h-BN in BN[Bmim][Tf2N]
Atomic Charge (e)
Atomic Number

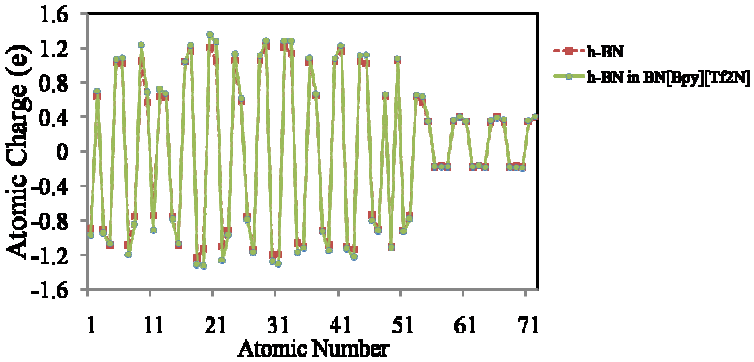

[Bpy][BF4]
[Bpy][BF4] after adsorption
Atomic Charge (e)
Atomic Number

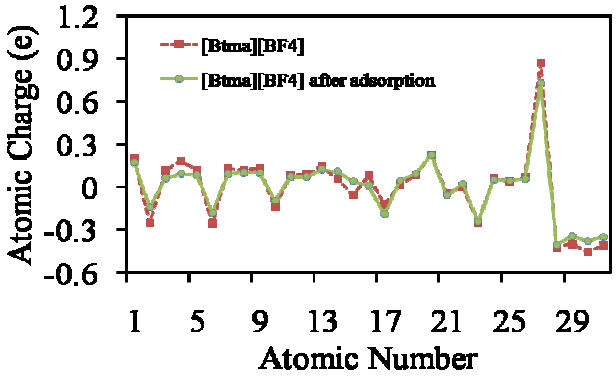

h-BN
h-BN in BN[Bpy][BF4]
Atomic Charge (e)
Atomic Number

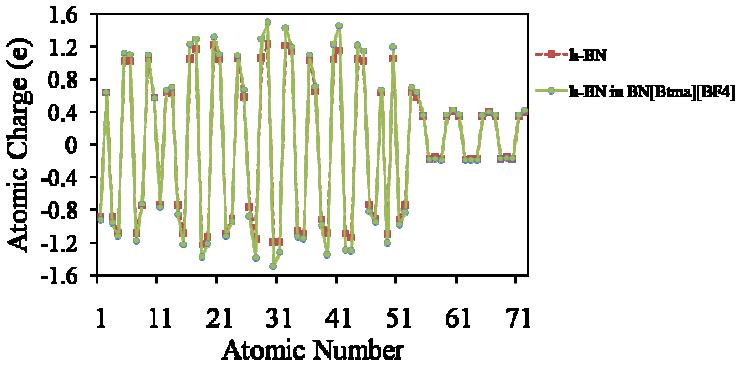

[Bpy][PF6]
[Bpy][PF6] after adsorption
Atomic Charge (e)
Atomic Number

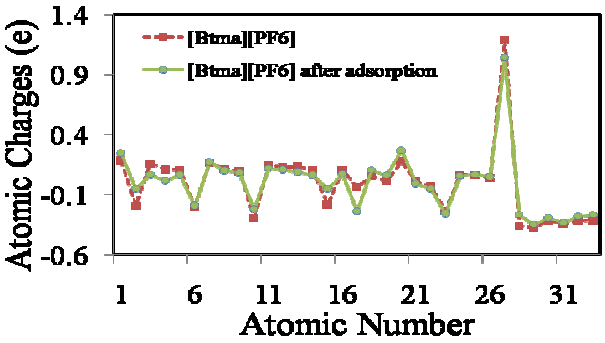

h-BN
h-BN in BN[Bpy][PF6]
Atomic Charge (e)
Atomic Number

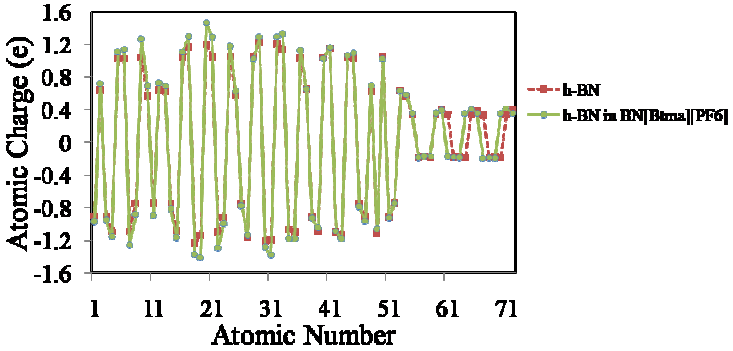

[Bpy][Tf2N]
[Bpy][Tf2N] after adsorption
Atomic Charge (e)
Atomic Number


h-BN
h-BN in BN[Bpy][Tf2N]
Atomic Charge (e)
Atomic Number


[Btma][BF4]
[Btma][BF4] after adsorption
Atomic Charge (e)
Atomic Number


h-BN
h-BN in BN[Btma][BF4]
Atomic Charge (e)
Atomic Number


[Btma][PF6]
[Btma][PF6] after adsorption
Atomic Charges (e)
Atomic Number


h-BN
h-BN in BN[Btma][PF6]
Atomic Charge (e)
Atomic Number

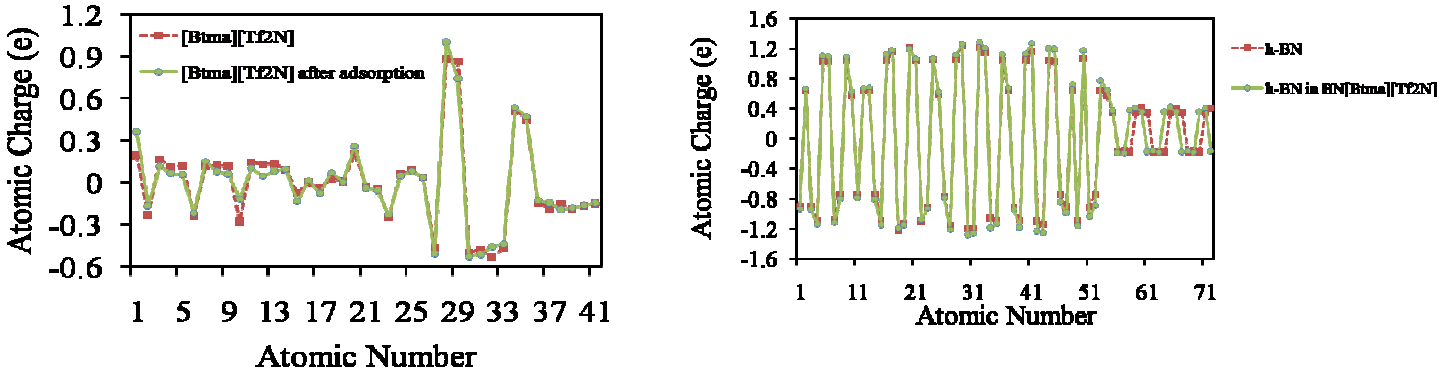


Figure S2. Comparison between the atomic charges obtained by using CHelpG analysis before and after adsorption of [Bmim][Y], [Bpy][Y], and [Btma][Y] (Y = BF_4^-, PF_6^-, and Tf_2N^-) on the *h*-BN surface at the M06-2X/cc-pVDZ level of theory.