Electronic supplementary information (ESI)

Interfacial interactions and structures of protic ionic liquids on graphite surface: a first-principles study and comparison with aprotic ionic liquids

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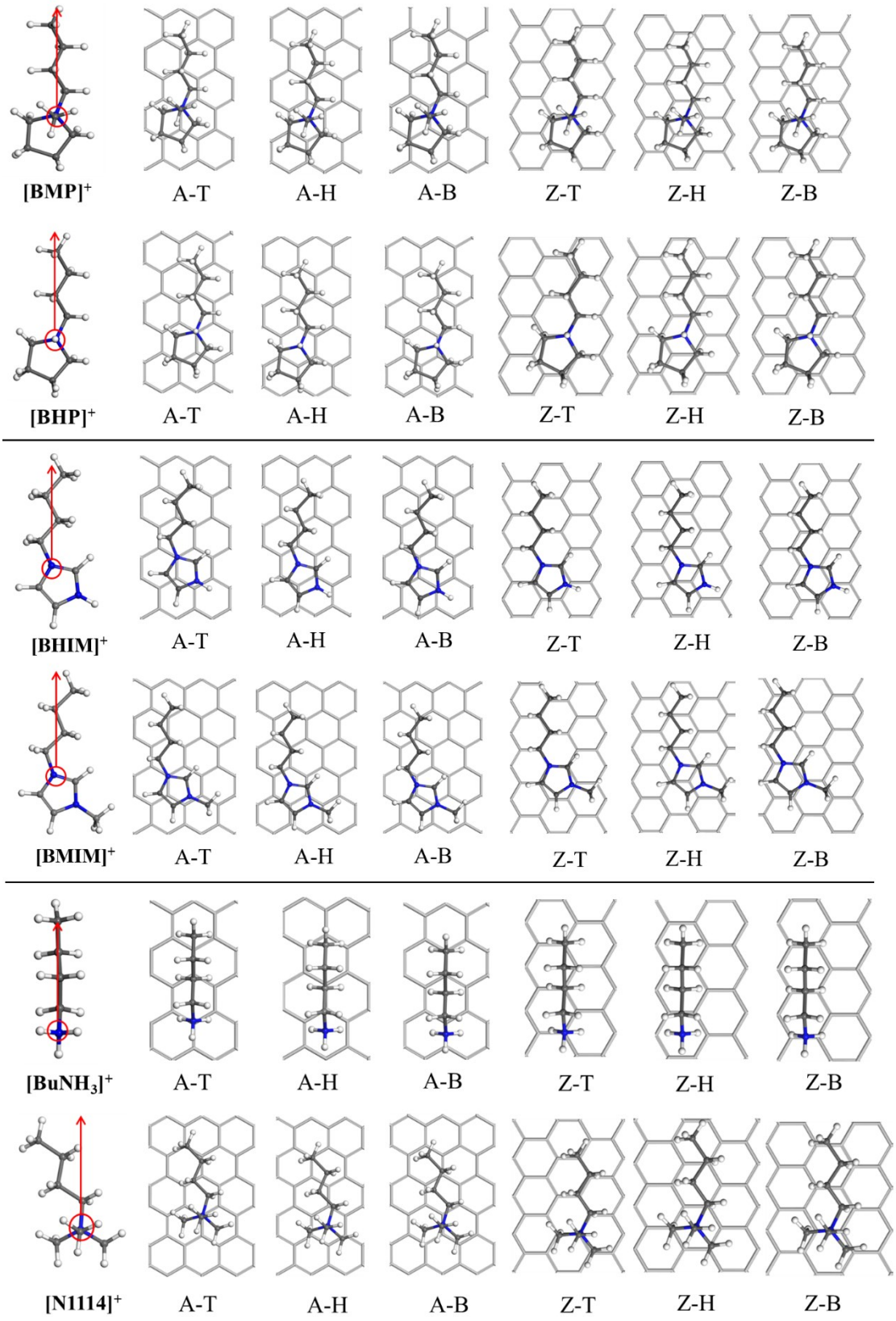

Fig. S1 Optimized structures for the isolated cations adsorbed at three different sites (T, H, B) on graphite with the butyl chain along armchair (A) and zigzag (Z) axes.

Table S1 The adsorption energies (kcal/mol) of the six configurations for the isolated cations[a]

E_{ads}	Armchair axis			Zigzag axis		
	Top	Hollow	Bridge	Top	Hollow	Bridge
$[BHP]^+$	-103.66	-102.86	-103.40	-102.98	-102.87	-103.45
$[BMP]^+$	-103.24	-102.79	-103.34	-102.58	-102.78	-103.19
$[BHIM]^+$	-103.65	-104.36	-103.86	-103.27	-104.49	-103.56
$[BMIM]^+$	-104.77	-104.82	-104.98	-104.35	-104.95	-104.08
$[BuNH_3]^+$	-104.12	-105.01	-103.63	-104.07	-105.40	-103.61
$[N1114]^+$	-101.81	-101.31	-101.37	-101.06	-100.97	-101.17

Table S2 Electronic charges (a.u.) of the six adsorption systems including the $[NO_3]$ anion[a]

Systems	$[BHP][NO_3]$	$[BMP][NO_3]$	$[BHIM][NO_3]$	$[BMIM][NO_3]$	$[BuNH_3][NO_3]$	$[N1114][NO_3]$
q_{CT}	0.02	-0.07	0.03	-0.11	0.03	-0.07
q_{anion}	-0.19	-0.18	-0.22	-0.21	-0.20	-0.18
q_{cation}	0.21	0.12	0.24	0.10	0.23	0.10
Δq_{anion}	0.00	-0.11	0.00	-0.12	0.04	-0.09
Δq_{cation}	0.02	0.04	0.03	0.01	-0.01	0.02

[a]q_{CT} represents the amount of charge transfer between the graphite surface and the adsorbed ILs; q_{anion} and q_{cation} are the charges of anion and cation on the surface; Δq_{anion} and Δq_{cation} are the charge changes of anion and cation upon the adsorption of ILs on graphite.