Electronic Supplementary Material for PCCP

Supplementary information

Molecular dynamics simulation of the electrochemical interface between graphite surface and ionic liquid [BMIM][PF_6]

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Schematic structures and AMBER atom types for the $[BMIM]^+$ cation and $[PF_6]^-$ anion. The numbers represent partial atomic charges (in units of *e*) as obtained by the ESP methodology:

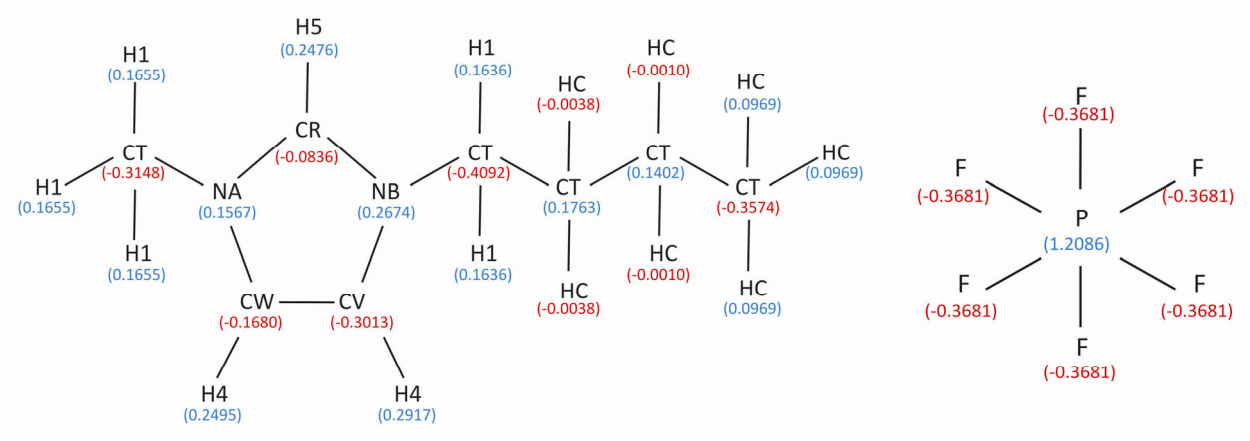

Table of the potential parameters

Bond stretching:

$$E_{bond} = \sum_{bonds} K_r (r - r_{eq})^2$$

Bond	K_r, kcal/(mol Å^2)	r_{eq}, Å
CR-NB	488	1.335
NB-CV	410	1.394
CV-CW	520	1.370
CW-NA	427	1.381
CT-CT	310	1.526
CR-NA	477	1.343
NB-CT	337	1.475
NA-CT	337	1.475
CT-H1	340	1.090
CV-H4	367	1.080
CW-H4	367	1.080
CT-HC	340	1.090
CR-H5	367	1.080

Angle bending:

$$E_{angle} = \sum_{angles} K_\theta (\theta - \theta_{eq})^2$$

Angle	K_θ, kcal/(mol rad^2)	θ_{eq}, degree
NB-CR-NA	70	120
NB-CR-H5	35	120
NA-CR-H5	35	120
CR-NB-CV	70	117
CR-NB-CT	70	125.8
CV-NB-CT	70	125.8
NB-CV-CW	70	106.2
NB-CV-H4	35	120
CW-CV-H4	35	120
CV-CW-NA	70	106.2
CV-CW-H4	35	120
NA-CW-H4	35	120
CR-NA-CW	70	120
CW-NA-CT	70	125.8
CR-NA-CT	70	125.8
NB-CT-CT	50	109.5
CT-CT-H1	50	109.5
NB-CT-H1	50	109.5
H1-CT-H1	35	109.5
CT-CT-CT	40	109.5
CT-CT-HC	50	109.5
HC-CT-HC	35	109.5

Torsion:

$$E_{torsion} = \sum_{dihedrals} \frac{V_n}{2}\left(1+\cos\left(n\varphi-\gamma\right)\right)$$

Dihedral	$V_n/2$, kcal/mol	γ,degree	n
X-CT-CT-X	0.156	0	3
X-CT-NB-X	0.00	0	2
X-CT-NA-X	0.00	0	2
X-X-CR-H5	1.1	180	2
X-X-CW-H4	1.1	180	2
X-X-CV-H4	1.1	180	2

VDW interaction:

$$E_{VDW} = \sum_{i<j} \varepsilon_{ij}\left(\frac{R_{ij}^{*\,12}}{R_{ij}^{\;12}} - 2\frac{R_{ij}^{*\,6}}{R_{ij}^{\;6}}\right),\ R_{ij}^{*} = R_i^{*} + R_j^{*},\ \varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j}$$

Atom type	R_i^*, Å	ε_i, kcal/mol
CT	1.9080	0.1094
HC	1.4870	0.0157
H1	1.3870	0.0157

H4	1.4090	0.0150
H5	1.3590	0.0150
CR	1.9080	0.0860
CV	1.9080	0.0860
CW	1.9080	0.0860
NA	1.8240	0.1700
NB	1.8240	0.1700
P	2.1000	0.2000
F	1.7500	0.0610

Electrostatic and van der Waals interactions are only calculated between atoms in different molecules or for atoms in the same molecule separated by at least three bonds. Those non-bonded interactions separated by exactly three bonds are reduced by the application of a scale factor.

Electrostatic scale factor: 1/1.2

VDW scale factor: 1/2