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Supplementary Information

Theoretical Study on the Structure and Electronic Properties of Alkylimidazolium Iodide Ionic Liquids: The Effect of Alkyl Chain Length

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Table S1. Selected partial charges from NBO analysis for $[C_n mim]^+$, n=4–8, at the MP2/DGDZVP level.

	$[C_4mim]^+$	**$[C_5mim]^+$**	**$[C_6mim]^+$**	**$[C_7mim]^+$**	**$[C_8mim]^+$**
N1	-0.362	-0.362	-0.361	-0.361	-0.361
C2	0.288	0.288	0.287	0.287	0.287
N3	-0.365	-0.365	-0.365	-0.365	-0.342
C4	0.012	0.011	0.011	0.011	0.011
C5	0.009	0.009	0.009	0.009	0.009
C6	-0.342	-0.342	-0.342	-0.342	-0.342
C7	-0.162	-0.161	-0.160	-0.160	-0.160
C8	-0.400	-0.395	-0.394	-0.394	-0.394
C9	-0.379	-0.391	-0.387	-0.386	-0.385
C10	-0.580	-0.373	-0.385	-0.380	-0.379
C11	–	-0.582	-0.374	-0.386	-0.381
C12	–	–	-0.581	-0.373	-0.385
C13	–	–	–	-0.581	-0.373
C14	–	–	–	–	-0.581
H15	0.237	0.237	0.237	0.237	0.237
H16	0.245	0.244	0.244	0.244	0.244
H17	0.245	0.245	0.245	0.245	0.245
C2–H15	0.525	0.525	0.524	0.524	0.524
C4–H16	0.257	0.255	0.255	0.255	0.255
C5–H17	0.254	0.254	0.254	0.254	0.254

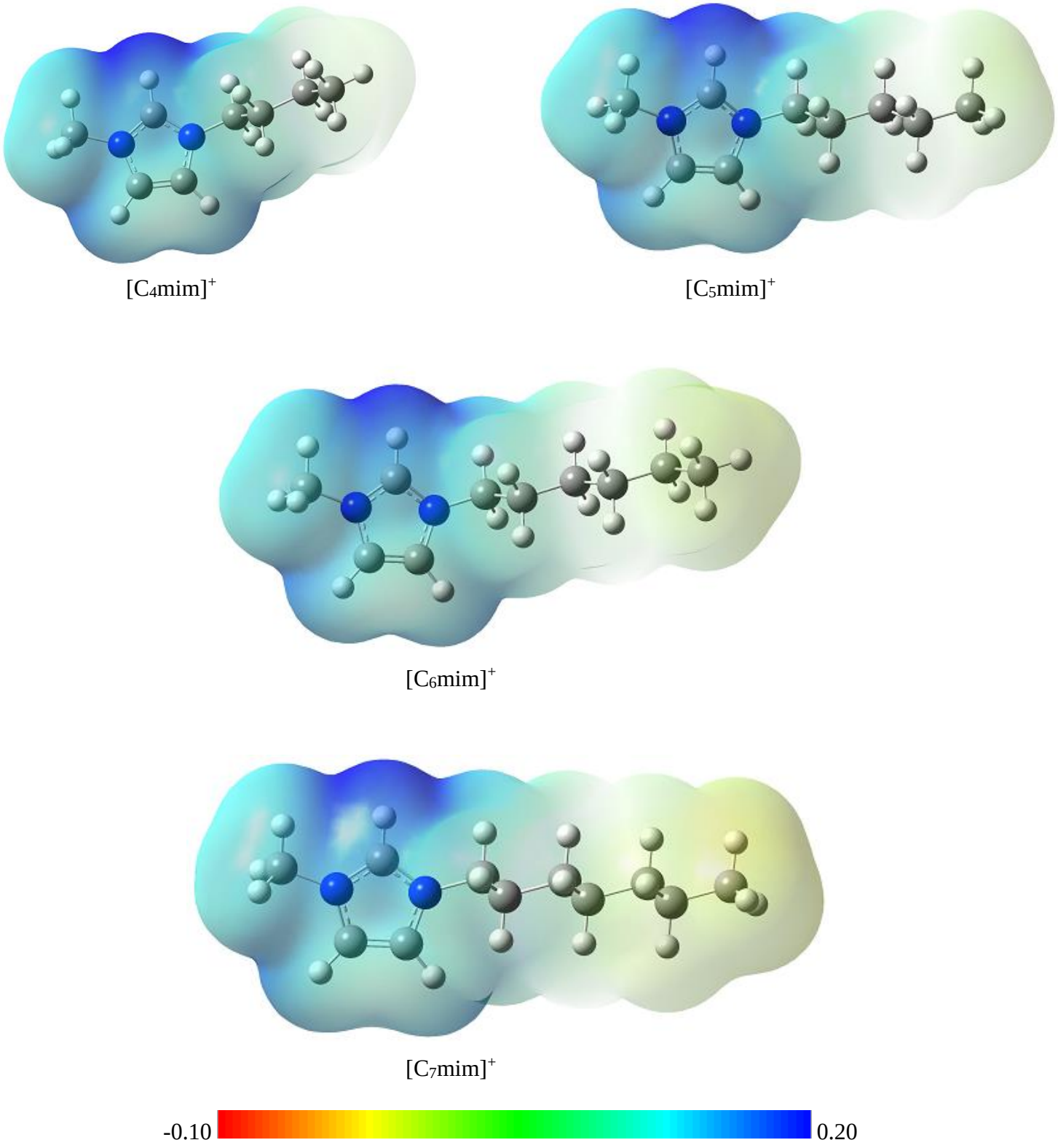
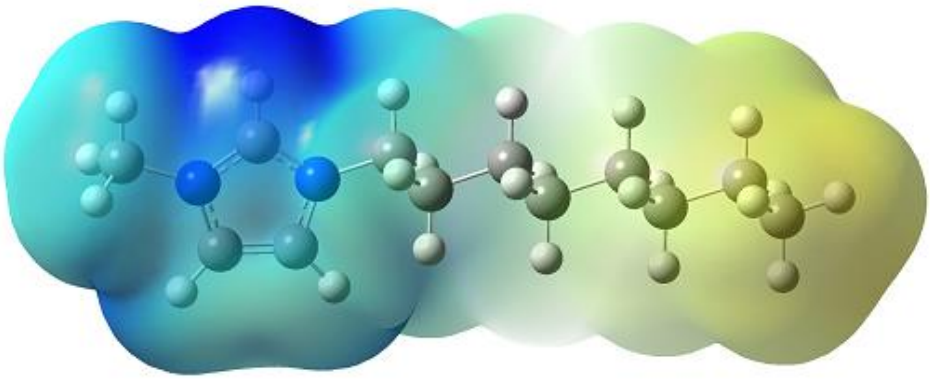


Figure S1. The obtained MEP maps for $[C_nmim]^+$, n=4–8.



$[C_8mim]^+$

Figure S1. Continued.

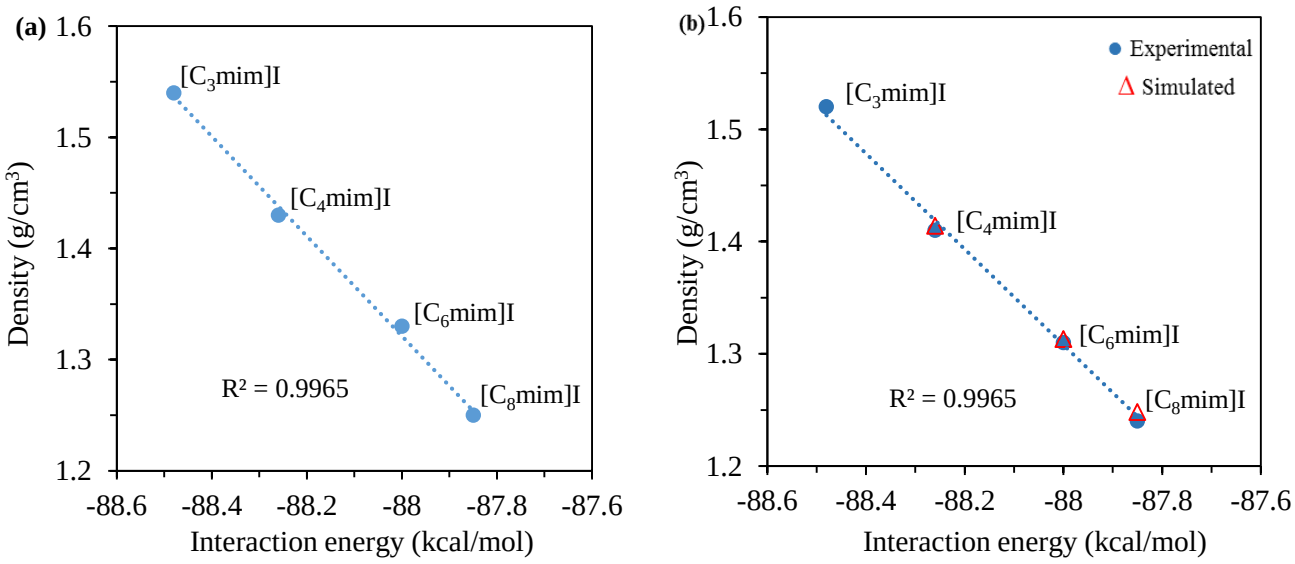


Figure S2. Correlation between interaction energy calculated at the MP2/6-311++G(d,p)[def2-QZVPP] level and density at **(a)** 308 K and **(b)** 323 K.

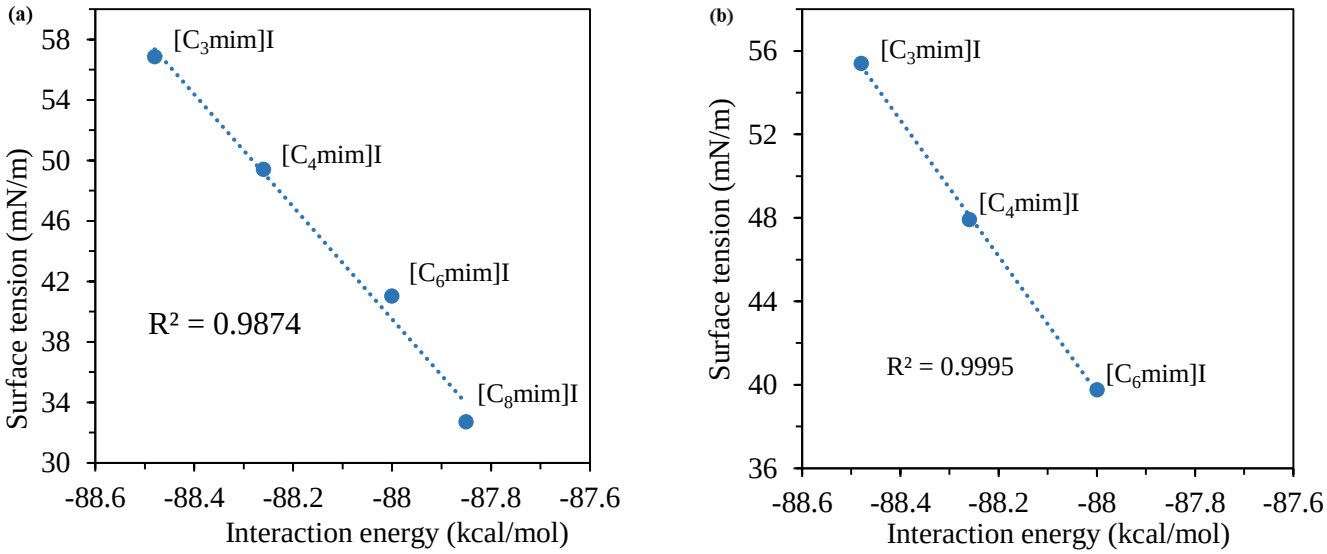


Figure S3. Correlation between interaction energy calculated at the MP2/6-311++G(d,p)[def2-QZVPP] level and experimental surface tension at **(a)** 298 K and **(b)** 323 K.

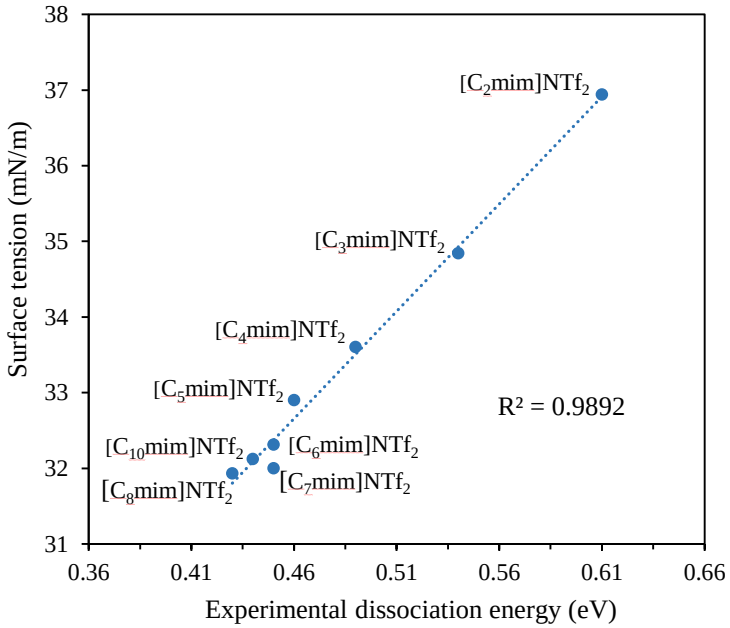


Figure S4. Correlation between the dissociation energies obtained by mass spectrometry experiments[1] and experimental surface tensions[2] at 293.15 K.

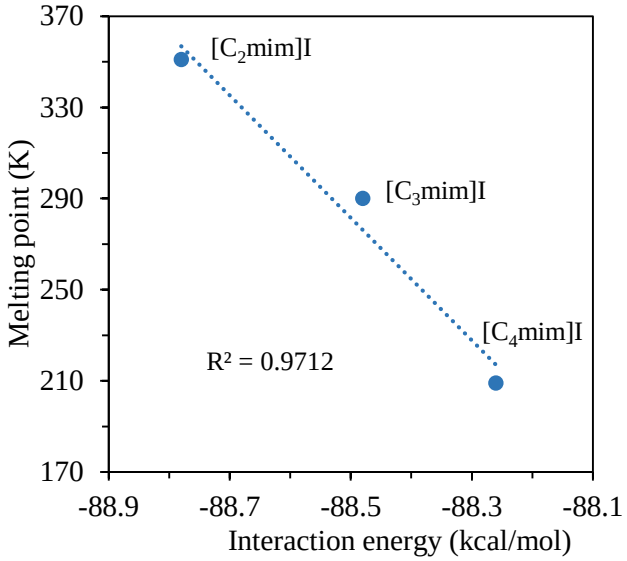


Figure S5. Correlation between interaction energy calculated at the MP2/6-11++G(d,p)[def2-QZVPP] level and experimental melting point for the [$C_n$mim]I ILs, with $n \leq 4$.

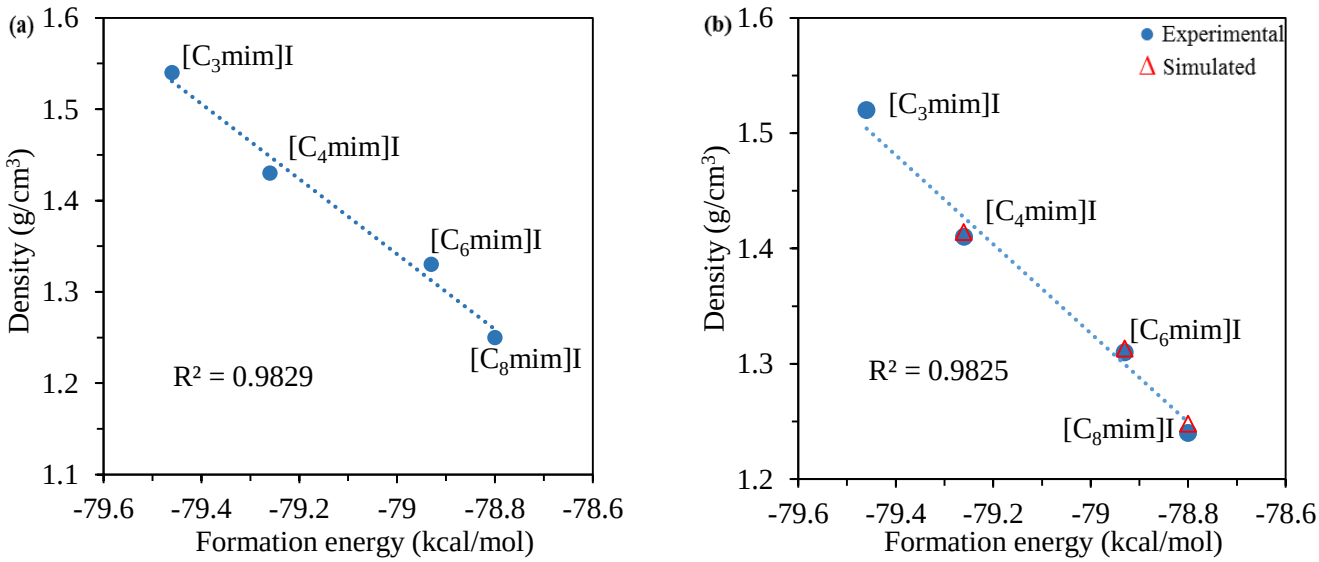


Figure S6. Correlation between formation energy calculated at the MP2/DGDZVP level and density at **(a)** 308 K and **(b)** 323 K.

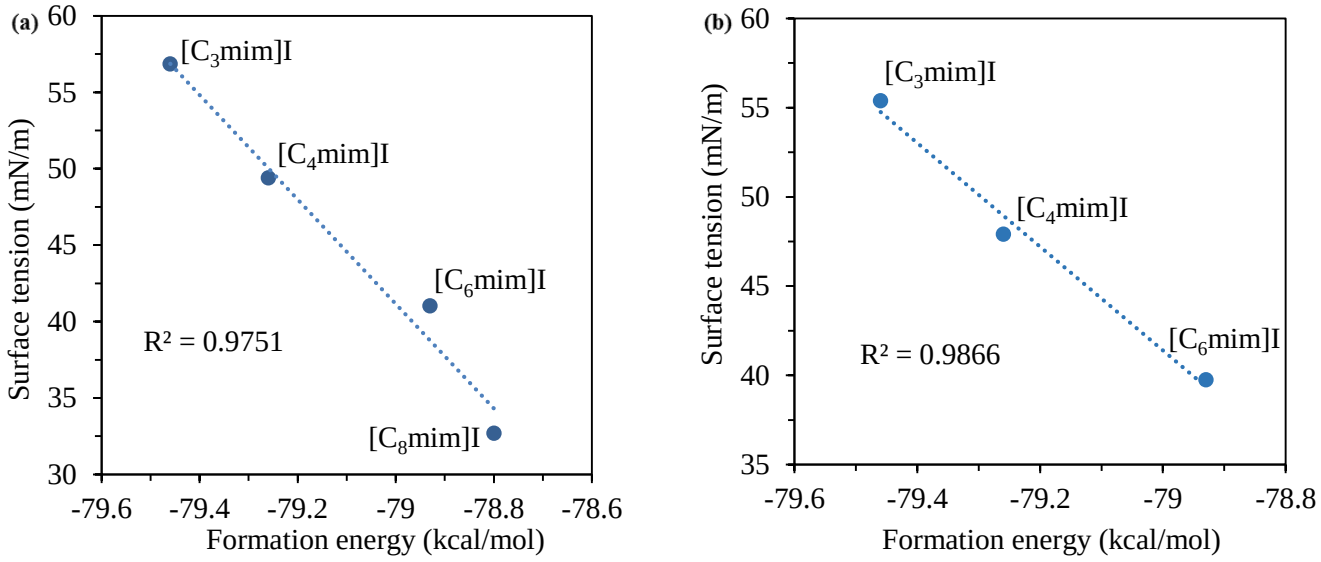


Figure S7. Correlation between formation energy calculated at the MP2/DGDZVP level and experimental surface tension at **(a)** 298 K and **(b)** 323 K.

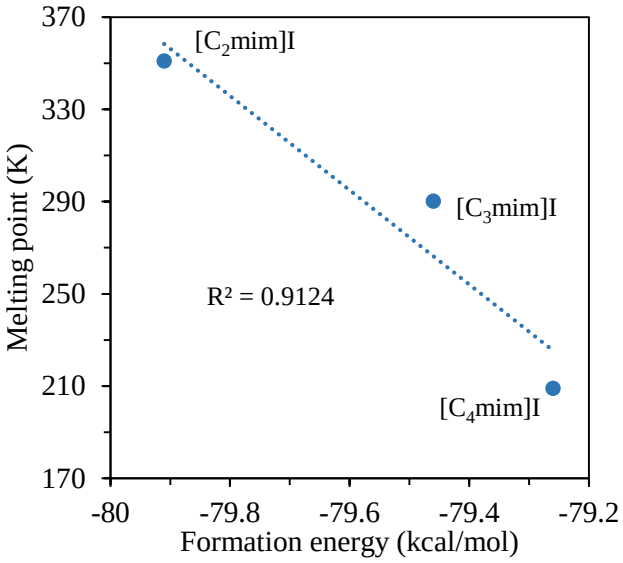


Figure S8. Correlation between formation energy calculated at the MP2/DGDZVP level and experimental melting point for the [C$_n$mim]I ILs, with $n \leq 4$.

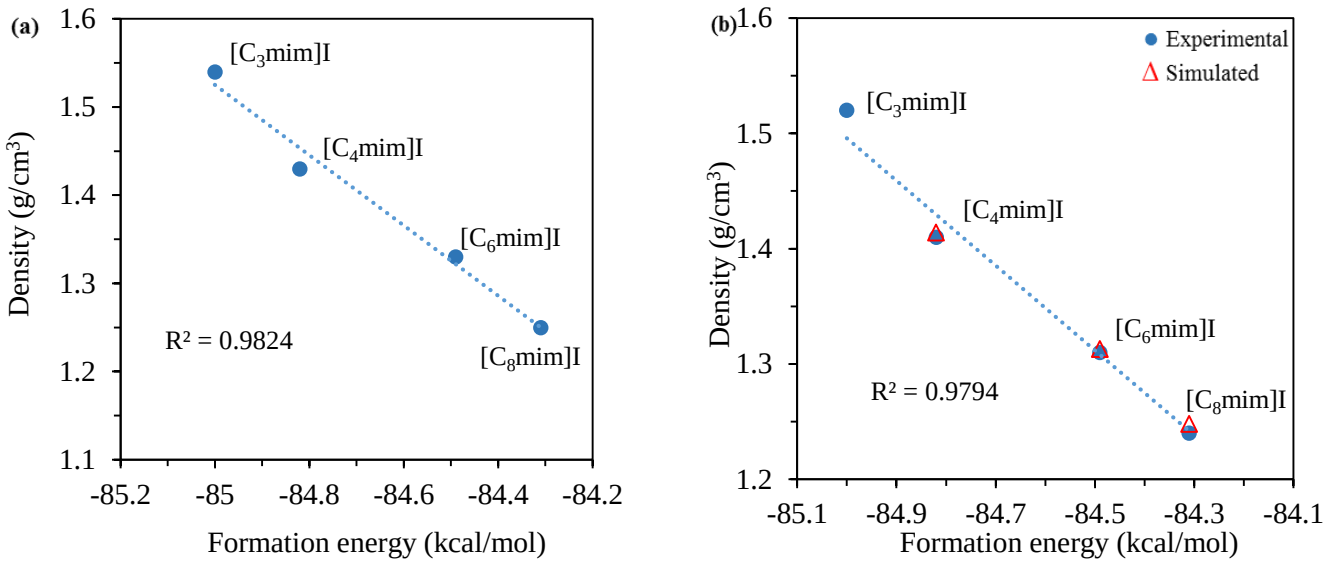


Figure S9. Correlation between formation energy calculated at the MP2/6-311++G(d,p)[def2-QZVPP] level and density at **(a)** 308 K and **(b)** 323 K.

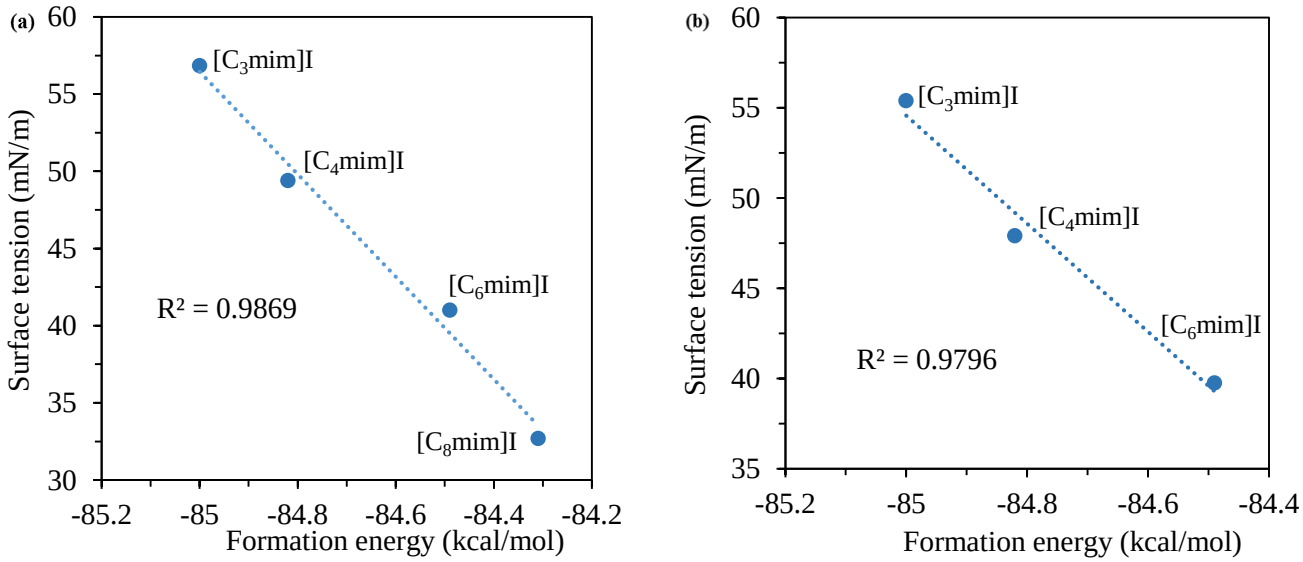


Figure S10. Correlation between formation energy calculated at the MP2/6-311++G(d,p)[def2-QZVPP] level and experimental surface tension at **(a)** 298 K and **(b)** 323 K.

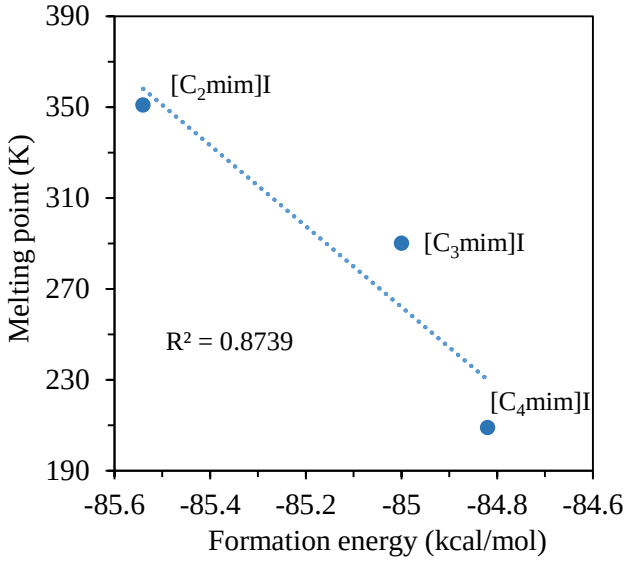


Figure S11. Correlation between formation energy calculated at the MP2/6-11++G(d,p)[def2-QZVPP] level and experimental melting point for the [$C_n$mim]I ILs, with $n \leq 4$.

References

1 A. M. Fernandes, M. A. A. Rocha, M. G. Freire, I. M. Marrucho, J. A. P. Coutinho and L. M. N. B. F. Santos, *J. Phys. Chem. B*, 2011, **115**, 4033–4041.

2 P. J. Carvalho, M. G. Freire, I. M. Marrucho, A. J. Queimada and J. A. P. Coutinho, *J. Chem. Eng. Data*, 2008, **53**, 1346–1350.