Supplementary Information (SI) for Soft Matter.
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Supporting Information

Translational diffusion and isomerization reaction of a liquid crystal molecule at solid-liquid interface of ionic liquids studied by total internal reflection-transient grating spectroscopy

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Table S1. The diffusion coefficients of MBBA in the bulk phase K together with the values of density ρ and viscosity η. The standard deviation of viscosity is less than 4 % of the value.

Sample	ρ / g cm^{-3}	$D^{(b)}$ / 10^{-11} m^2 s^{-1}	η / mPa s
IL_3LC	-[a]	3.4 ± 0.1	52
IL_4LC	1.341	3.4 ± 0.1	65
IL_6LC	-[a]	4.6 ± 0.1	76
IL_8LC	1.253	3.6 ± 0.1	103
$IL_{10}LC$	-[a]	2.4 ± 0.1	115
$IL_{12}LC$	1.198	2.3 ± 0.0	146

a) not measured.

Table S2. The diffusion coefficients and reaction rates of MBBA near the interface together with the refractive index n_D and the water contamination after the TIR-TG measurements. The standard deviation of refractive index is approximately 0.02% of the value.

Sample	$D^{(i)}$ / 10^{-11} m^2 s^{-1}	$k_{ct}^{(i)}$ / s^{-1}	n_D	water content / ppm
IL_4LC	3.4 ± 0.1	11.5 ± 0.5	1.46	610
IL_6LC	4.2 ± 0.2	5.9 ± 1.3	-[a]	300
IL_8LC	3.9 ± 0.1	6.0 ± 0.6	1.46	570
$IL_{12}LC$	2.3 ± 0.1	12.5 ± 0.4	1.47	410

a) not measured.

Table S3. The surface tension γ and contact angle θ_c on sapphire for IL_nLCs, ILs, and MBBA.

Sample	γ / mN m^{-1}	θ_c / degree
IL_4LC	33.3 ± 0.1	11.8 ± 1.4
IL_8LC	32.1 ± 0.1	8.0 ± 0.4
$IL_{12}LC$	31.8 ± 0.1	7.2 ± 0.4
$[C_4mim][NTf_2]$	33.2[a]	15.7 ± 1.6
$[C_8mim][NTf_2]$	31.4[a]	10.3 ± 1.8
$[C_{12}mim][NTf_2]$	28.1[b]	8.8 ± 0.8
MBBA	34.3 ± 0.1	6.8 ± 1.0

a) Taken from ref. 1)

b) Taken from ref. 2)

Table S4. Number of cation, anion, and MBBA in the MD simulation.

System	Cation	Anion	MBBA
IL_4LC	1600	1600	400
IL_8LC	1400	1400	350
$IL_{12}LC$	1200	1200	300

Table S5. Density calculated by MD simulation $\rho^{(\mathrm{calc})}$ and relative deviation from the experimental value $\Delta\rho$.

System	$\rho^{(\mathrm{calc})}$ / g cm^{-3}	$\Delta\rho$ / %
IL_4LC	1.395 ± 0.002	$+4.0$
IL_8LC	1.307 ± 0.002	$+4.3$
$IL_{12}LC$	1.250 ± 0.003	$+4.3$

Table S6 Diffusion coefficients calculated by MD simulation $D^{(\mathrm{calc})}$ and corrected diffusion coefficient of MBBA $D_{\mathrm{MBBA}}^{(\mathrm{corr})}$ according to ref. 3).

	IL_4LC	IL_8LC	$IL_{12}LC$
$D_{\mathrm{MBBA}}^{(\mathrm{calc})}$ / 10^{-12} m^2 s^{-1}	8.8 ± 0.1	4.0 ± 0.1	1.6 ± 0.1
$D_{\mathrm{cation}}^{(\mathrm{calc})}$ / 10^{-12} m^2 s^{-1}	11 ± 0	2.9 ± 0.0	0.84 ± 0.04
$D_{\mathrm{anion}}^{(\mathrm{calc})}$ / 10^{-12} m^2 s^{-1}	8.0 ± 0.1	2.9 ± 0.1	0.99 ± 0.03
$D_{\mathrm{MBBA}}^{(\mathrm{corr})}$ / 10^{-12} m^2 s^{-1}	9.8	4.6	2.0

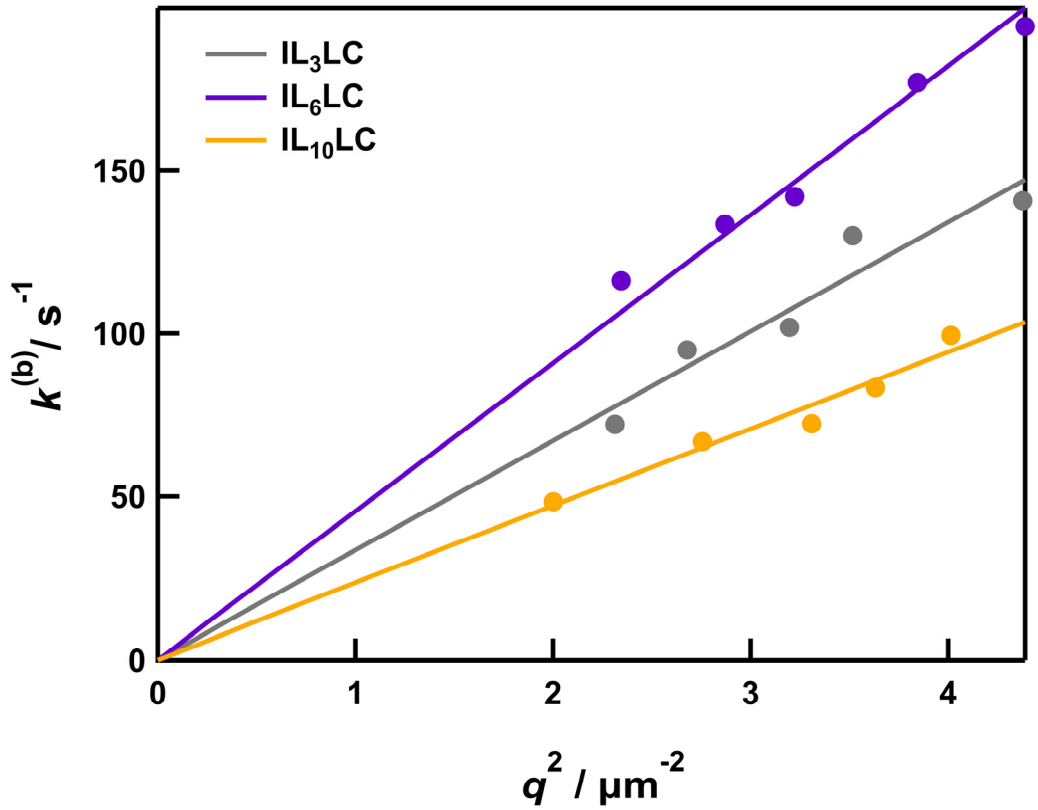

Fig. S1. Plot of the decay rate constants $k^{(b)}$ against q^2 for IL$_n$LC (n = 3, 6, and 10).

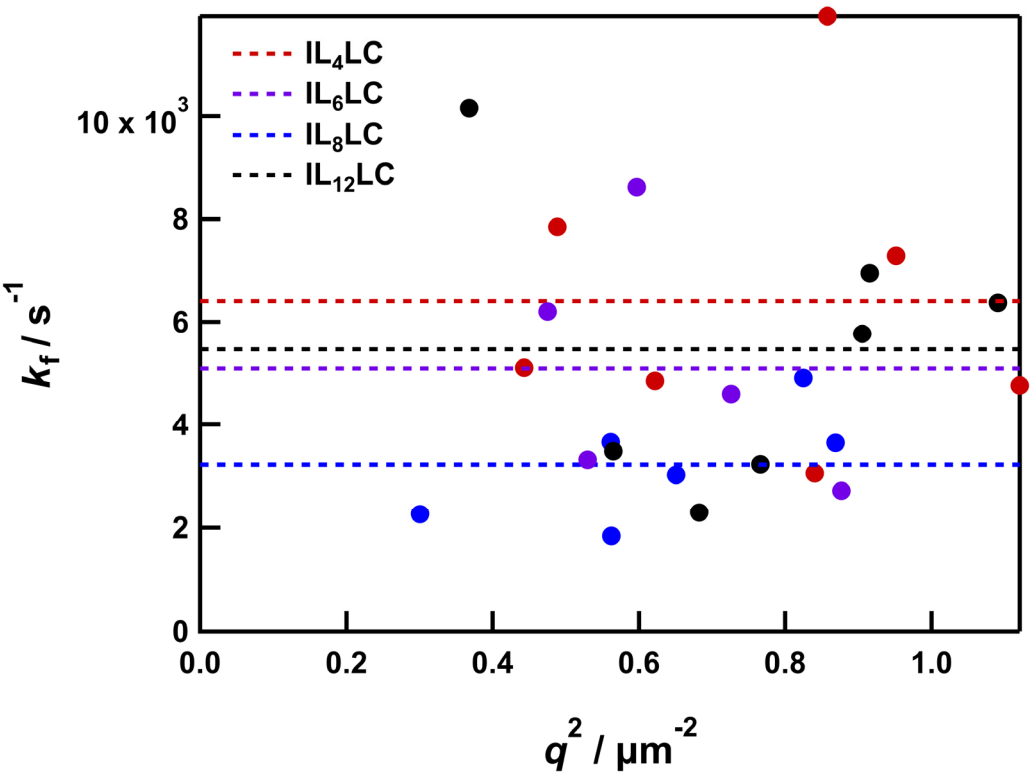

Fig. S2. Plot of the decay rate constants k_f against q^2 for each IL_nLC.

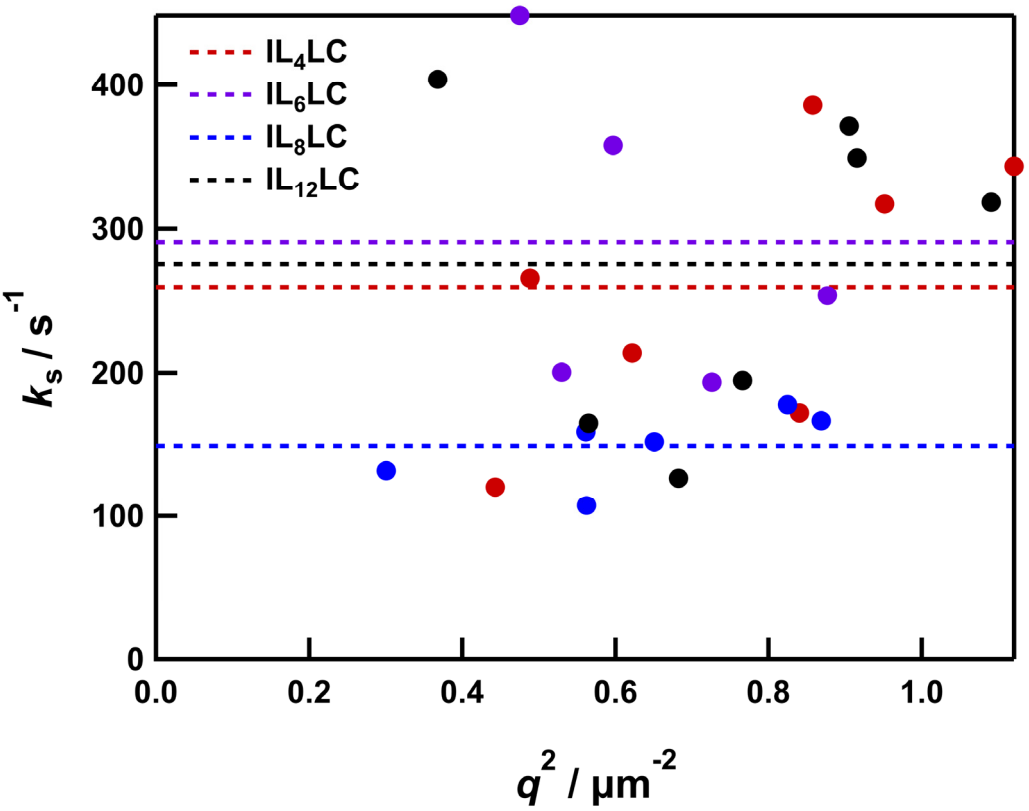

Fig. S3. Plot of the decay rate constants k_s against q^2 for each IL_nLC.

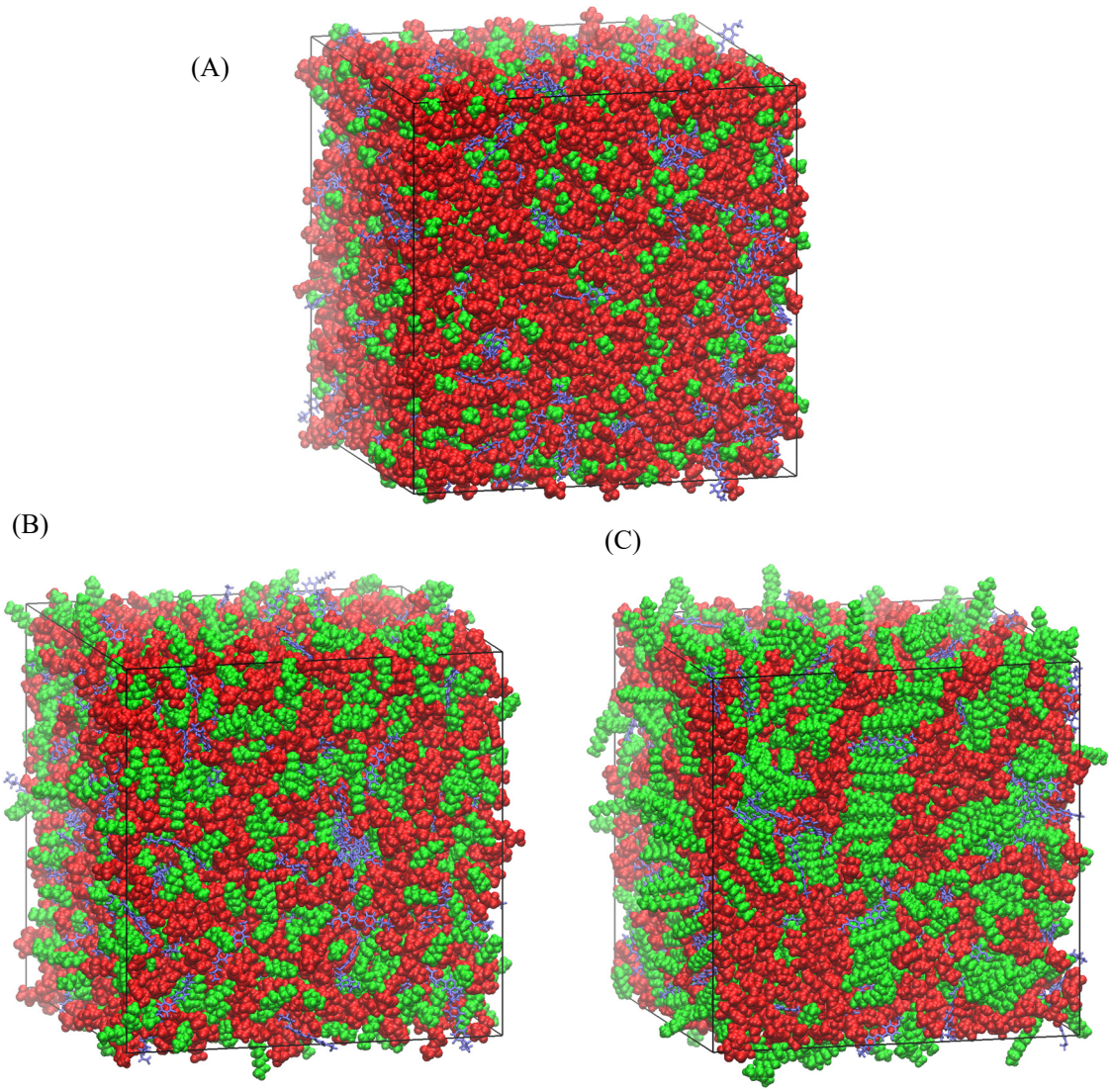

Fig. S4. Snapshots of (A) IL_4LC, (B) IL_8LC, and (C) $IL_{12}LC$. Polar and nonpolar domains are colored red and green, and MBBA is colored blue. The box size was 9.75 nm for IL_4LC, 9.82 nm for IL_8LC, and 9.84 nm for $IL_{12}LC$.

References

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