Electronic Supplementary Information (ESI)

Relationship between Force Curve Measured by Atomic Force Microscopy in Ionic Liquid and its Density Distribution on a Substrate

Ken-ichi Amano,^{a*} Yasuyuki Yokota,^b Takashi Ichii,^c Norio Yoshida,^d Naoya Nishi,^a Seiji Katakura,^a Akihito Imanishi,^e Ken-ichi Fukui,^e and Tetsuo Sakka^a

^a Department of Energy and Hydrocarbon Chemistry, Graduate School of Engineering, Kyoto University, Kyoto 615-8510, Japan.

E-mail: amano.kenichi.8s@kyoto-u.ac.jp

^b Surface and Interface Science Laboratory, RIKEN, Saitama 351-0198, Japan

^c Department of Materials Science and Engineering, Kyoto University, Kyoto, 606-8501, Japan

^d Department of Chemistry, Graduate School of Science, Kyushu University, Fukuoka 819-0395, Japan

^e Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University, 1-3 Machikaneyama, Toyonaka, Osaka 560-8531, Japan

Figure and Tables

OZ-HNC for the ionic liquid

(1) Calculation of bulk structure of a ionic liquid: Density distribution of cations around a cation, Density distribution of anions around a cation, Density distribution of cations around an anion, Density distribution of anions around an anion.

(2) Calculation of the solvation structures:

Density distribution of cations around a probe, Density distribution of anions around a probe, Density distribution of cations on a substrate, Density distribution of cations around a substrate.

(3) Calculation of mean force between the substrate and the probe.

If the probe is the ideal one, use Eq. (3), else use both Eq. (3) and Eq. (5). (The probe surface must be positively or negatively charged.)

(4) Reconstruction:

Density distribution of cations on a substrate, Density distribution of cations around a substrate.

Fig. S1 Overview of the calculation process.

$d_{\mathrm{P}}\left(\mathrm{m} ight)$	$\sigma_{\rm P}$ (C/nm ²)	C^*
$2d_0$	$\pm\sigma_0$	0.4356
$2d_0$	$\pm \sigma_0/2$	0.8553
$3d_0$	$\pm\sigma_0$	0.3088
$3d_0$	$\pm \sigma_0/2$	0.7944
$4d_0$	$\pm\sigma_0$	0.2431
$4d_0$	$\pm \sigma_0/2$	0.7459

Table S1 Values of C^* for conditions written in Fig. 7, where $\sigma_B = 0$. The value of C^* increases with increase in d_P . The value of C^* for large $|\sigma_P|$ is smaller than that for small $|\sigma_P|$.

Table S2 Values of C^* for conditions written in Fig. 8(a), where $\sigma_B = -\sigma_0$. The value of C^* decreases with increase in d_P . The value of C^* for large σ_P is larger than that for small σ_P .

$d_{\mathrm{P}}\left(\mathrm{m} ight)$	$\sigma_{\rm P} ({\rm C/nm^2})$	C^*
$2d_0$	$+\sigma_0$	0.8312
$2d_0$	$+\sigma_{0}/2$	0.4324
$3d_0$	$+\sigma_0$	0.5413
$3d_0$	$+\sigma_{0}/2$	0.2798
$4d_0$	$+\sigma_0$	0.4094
$4d_0$	$+\sigma_{0}/2$	0.2107

Table S3 Values of C^* for conditions written in Fig. 8(b), where $\sigma_B = -\sigma_0$. The value of C^* decreases with increase in d_P . The value of C^* for large $|\sigma_P|$ is larger than that for small $|\sigma_P|$.

$d_{\mathrm{P}}\left(\mathrm{m} ight)$	$\sigma_{\rm P}$ (C/nm ²)	<i>C</i> *
$2d_0$	$-\sigma_0$	0.8273
$2d_0$	$-\sigma_{0}/2$	0.4237
$3d_0$	$-\sigma_0$	0.5563
$3d_0$	$-\sigma_{0}/2$	0.2762
$4d_0$	$-\sigma_0$	0.4311
$4d_0$	$-\sigma_{0}/2$	0.2116