# Electronic Supplementary Information (ESI) 

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

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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.

Table S1 Values of $C^{*}$ for conditions written in Fig. 7, where $\sigma_{\mathrm{B}}=0$. The value of $C^{*}$ increases with increase in $d_{\mathrm{P}}$. The value of $C^{*}$ for large $\left|\sigma_{\mathrm{P}}\right|$ is smaller than that for small $\left|\sigma_{\mathrm{P}}\right|$.

| $d_{\mathrm{P}}(\mathrm{m})$ | $\sigma_{\mathrm{P}}\left(\mathrm{C} / \mathrm{nm}^{2}\right)$ | $C^{*}$ |
| :---: | :---: | :---: |
| $2 d_{0}$ | $\pm \sigma_{0}$ | 0.4356 |
| $2 d_{0}$ | $\pm \sigma_{0} / 2$ | 0.8553 |
| $3 d_{0}$ | $\pm \sigma_{0}$ | 0.3088 |
| $3 d_{0}$ | $\pm \sigma_{0} / 2$ | 0.7944 |
| $4 d_{0}$ | $\pm \sigma_{0}$ | 0.2431 |
| $4 d_{0}$ | $\pm \sigma_{0} / 2$ | 0.7459 |

Table S2 Values of $C^{*}$ for conditions written in Fig. 8(a), where $\sigma_{\mathrm{B}}=-\sigma_{0}$. The value of $C^{*}$ decreases with increase in $d_{\mathrm{P}}$. The value of $C^{*}$ for large $\sigma_{\mathrm{P}}$ is larger than that for small $\sigma_{\mathrm{P}}$.

| $d_{\mathrm{P}}(\mathrm{m})$ | $\sigma_{\mathrm{P}}\left(\mathrm{C} / \mathrm{nm}^{2}\right)$ | $C^{*}$ |
| :---: | :---: | :---: |
| $2 d_{0}$ | $+\sigma_{0}$ | 0.8312 |
| $2 d_{0}$ | $+\sigma_{0} / 2$ | 0.4324 |
| $3 d_{0}$ | $+\sigma_{0}$ | 0.5413 |
| $3 d_{0}$ | $+\sigma_{0} / 2$ | 0.2798 |
| $4 d_{0}$ | $+\sigma_{0}$ | 0.4094 |
| $4 d_{0}$ | $+\sigma_{0} / 2$ | 0.2107 |

Table S3 Values of $C^{*}$ for conditions written in Fig. 8(b), where $\sigma_{\mathrm{B}}=-\sigma_{0}$. The value of $C^{*}$ decreases with increase in $d_{\mathrm{P}}$. The value of $C^{*}$ for large $\left|\sigma_{\mathrm{P}}\right|$ is larger than that for small $\left|\sigma_{\mathrm{P}}\right|$.

| $d_{\mathrm{P}}(\mathrm{m})$ | $\sigma_{\mathrm{P}}\left(\mathrm{C} / \mathrm{nm}^{2}\right)$ | $C^{*}$ |
| :---: | :---: | :---: |
| $2 d_{0}$ | $-\sigma_{0}$ | 0.8273 |
| $2 d_{0}$ | $-\sigma_{0} / 2$ | 0.4237 |
| $3 d_{0}$ | $-\sigma_{0}$ | 0.5563 |
| $3 d_{0}$ | $-\sigma_{0} 2$ | 0.2762 |
| $4 d_{0}$ | $-\sigma_{0}$ | 0.4311 |
| $4 d_{0}$ | $-\sigma_{0} 2$ | 0.2116 |

