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[J. Chem. Phys. 150, 044701 (2019)]

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We found a mis-implementation of the solid–liquid interfacial energy by the thermodynamic integration method in Eqs. (11) and (12) in the original article,¹ and related to this, Figs. 7 and 8 were revised. The changes in the these figures due to the corrections of Eqs. (11) and (12) were negligibly small, and the main conclusion is not affected by the corrections.

In addition, the unit in Table I and the value of γ_{LV} as typos were also corrected. The changes are as follows:

Page 6, line 3:

Hence, the difference of the SL interfacial Gibbs free energy $\Delta G_{SL} \equiv G_{SL}|_{\lambda=1^-} - G_{SL}|_{\lambda=0}$ between systems at $\lambda = 0$ and $\lambda = 1^-$ under constant NpT was related to the difference in the surface interfacial energies as

$$W_{SL} \equiv \frac{\Delta G_{SL}}{A} = \gamma_{S0} + \gamma_{L0} - \gamma_{SL} \\ \approx \gamma_{S0} + \gamma_{LV} - \gamma_{SL}, \quad (11)$$

where the vacuum phase is denoted by subscript “0” and γ_{S0} and γ_{L0} are the solid–vacuum and liquid–vacuum interfacial energies per unit area. Note that γ_{L0} was substituted by the liquid–vapor interfacial tension γ_{LV} in the final approximation considering that the vapor density was negligibly small. The work of adhesion W_{SL} was defined by the minimum work needed to strip the liquid from the solid surface per area under constant NpT .

Using the NpT canonical ensemble associated with the Gibbs free energy G , the difference of the SL interfacial Gibbs free energy ΔG_{SL} in Eq. (11) was calculated through the following TI:

$$\begin{aligned} \Delta G_{SL} &= \Delta G - Ap_{set}(\langle z_p|_{\lambda=1^-} \rangle - \langle z_p|_{\lambda=0} \rangle), \\ \Delta G &= \int_0^{1^-} \frac{dG(\lambda)}{d\lambda} d\lambda = \int_0^{1^-} \left\langle \frac{\partial H}{\partial \lambda} \right\rangle d\lambda \\ &= - \int_0^{1^-} \left\langle \sum_{i \in \text{fluid}} \sum_{j \in \text{wall}}^{N_w} \Phi_{fw}^{LJ} \right\rangle d\lambda, \end{aligned} \quad (12)$$

where H is the Hamiltonian, i.e., internal energy of the system and N_w is the number of wall molecules. The ensemble average was substituted by the time average in the simulation and was denoted by the angular brackets.

Note that to obtain ΔG_{SL} , the work exerted on the piston $Ap_{set}(\langle z_p|_{\lambda=1^-} \rangle - \langle z_p|_{\lambda=0} \rangle)$ was subtracted from the change of the Gibbs free energy ΔG of the whole system including the piston in Eq. (12).

Page 11, Fig. 7:

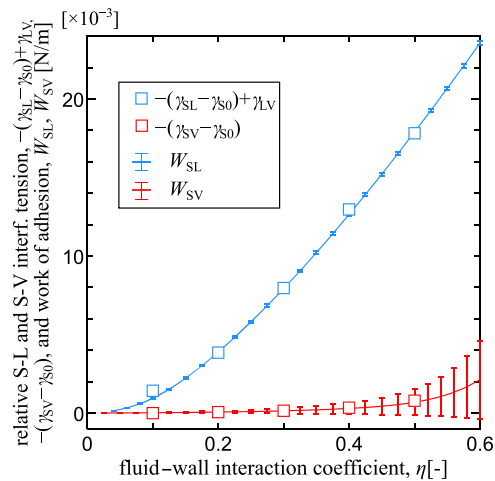


FIG. 7. Comparison between relative interfacial tensions obtained from the mechanical route and work of adhesion for flat SL and SV interfaces obtained by the DS method as a thermodynamic route. Considering the difference of the definitions, relative interfacial tensions $\gamma_{SL} - \gamma_{S0}$ and $\gamma_{SV} - \gamma_{S0}$ are shown as $-(\gamma_{SL} - \gamma_{S0}) + \gamma_{LV}$ and $-(\gamma_{SV} - \gamma_{S0})$, respectively, where $\gamma_{LV} = 11.3 \times 10^{-3}$ N/m is added to $-(\gamma_{SL} - \gamma_{S0})$. The value of γ_{LV} was obtained from a standard simulation system with a planer liquid-vapor interface.^{20,27} The error bars were obtained from the standard deviation.

Page 11, Fig. 8:

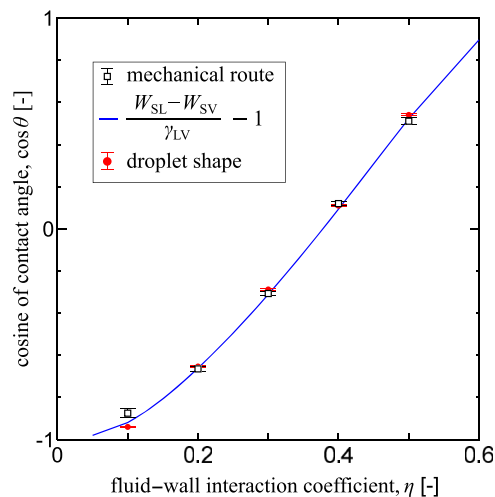


FIG. 8. Comparison between the apparent contact angle obtained from the droplet system and expected contact angle from the interfacial tensions obtained through mechanical and thermodynamic routes.

Page 5, Table I:

TABLE I. Simulation parameters and their corresponding non-dimensional values.

Property	Value	Unit	Non-dim. value
p_{set} (DS-SL)	1.00×10^6	Pa	2.35×10^{-2}

Page 11, line 9 following Eq. (38):

The value of $\gamma_{LV} = 11.3 \times 10^{-3}$ N/m was also used as well.

REFERENCE

¹Y. Yamaguchi, H. Kusudo, D. Surblys, T. Omori, and G. Kikugawa, *J. Chem. Phys.* **150**, 044701 (2019).