


Erratum: “A coarse-grained polymer model for studying the glass transition” [J. Chem. Phys. 150, 091101 (2019)]

Cite as: J. Chem. Phys. 150, 159902 (2019); <https://doi.org/10.1063/1.5097690>

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In the original article,¹ one error and several typos have been noticed.

In Fig. 1(a), the WCA excluded volume interaction potential

$$U_{\text{WCA}}(r) = \begin{cases} 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 + \frac{1}{4} \right], & r \leq r_{\text{cut}} \\ 0, & r > r_{\text{cut}} \end{cases}$$

with $r_{\text{cut}} = 2^{1/6}\sigma$ was not plotted correctly. The correct one [Fig. 1(a)] is reported below.

Page 2, left column, line 7 from bottom:

The text: “at $r = 5.0$ ” should be corrected to “at $r = 2.5\sigma$.”

Page 2, right column, line 7 below Eq. (2):

The text: “ $U_{\text{BEND}}(\theta)$ with $k_{\theta} = 1.5\epsilon$ ” should be corrected to “ $U_{\text{BEND}}^{(\text{old})}(\theta)$ with $k_{\theta} = 1.5\epsilon$.”

Figures 3(a) and 3(c):

The label: “ $U_{\text{BEND}}(\theta)$ ” should be corrected to “ $U_{\text{BEND}}^{(\text{old})}(\theta)$.”

Figures 3(b) and 3(d):

The label: “ $U_{\text{BEND}}^{(\text{new})}(\theta)$ ” should be corrected to “ $U_{\text{BEND}}(\theta)$.”

Figure 4(b):

The label: “ $U_{\text{BEND}}^{(\text{new})}(\theta)$ ” should be corrected to “ $U_{\text{BEND}}(\theta)$.”

These corrections have no impact on the results and the conclusion of this paper.

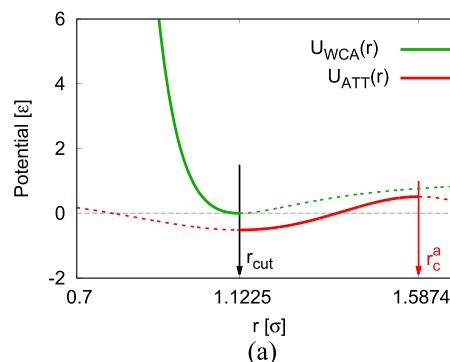


FIG. 1. (a) Nonbonded and short-range repulsive potential $U_{\text{WCA}}(r)$ and attractive potential $U_{\text{ATT}}(r)$ with $\alpha = 0.5145\epsilon$ [Eq. (1) in Ref. 1] plotted as a function of distance r .

REFERENCE

¹H.-P. Hsu and K. Kremer, J. Chem. Phys. 150, 091101 (2019).