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## **Erratum**

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## ERRATUM

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### MOLECULAR DYNAMICS MODELLING OF POLYMER MATERIALS

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An error has come to light in the method we described in the Appendix of the above paper concerning the contribution to the pressure tensor from the “bonding forces” i.e. those forces which maintain the bond length constraints and those derived from the valence angle and torsional angle potential in our model polymer. The correct procedure at step (9) of our algorithm is to use the set of coordinates  $\mathbf{r}(t)$  which describe the continuous chain i.e. where  $(\mathbf{r}_{i+1} - \mathbf{r}_i)^2 = b_0^2$  and **not** the positions of the sites within the primary cell. So step (9) in the Appendix should read:

(9) Using the position of sites on the continuous chain compute the contribution to the pressure tensor from the bonded forces

$$V(t)\mathbf{P}_{bf}(t) = \sum_{i=1}^N \mathbf{r}_i(t)[\mathbf{f}_i(t) - \mathbf{f}_i^\phi(t)] \quad (\text{A14})$$

where  $\mathbf{f}_i$  is now the total force on a site including the forces of constraint, equation (A11). The forces due to the LJ potential are subtracted as their contribution has already been calculated, equation (A7). The use of the coordinates of the continuous chain for calculating  $\mathbf{P}_{bf}$  is essential to maintain consistency with those used in actually calculating the bonding forces.

Quantitatively the pressure was found to be  $\sim 1\text{--}2$  kbar higher when the corrected pressure calculation was used and this resulted in a drop in density of  $\sim 0.02 \text{ g cm}^{-3}$  when the  $N = 1000$  site sample was re-equilibrated at a constant pressure of 1 bar at  $T = 300 \text{ K}$ . In qualitative terms this error is unlikely to change the general conclusions of the paper.