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In the original article,¹ we simulate the most fine grained model of the confined polymer melts with the standard version of the ESPResSo++ package,^{2,3} sticking for technical reasons to periodic boundary conditions in all three spatial dimensions of the rectangular simulation box (L_x, L_y, L_z). The confinement is introduced by a wall with a repulsive potential located at $z = 0$ (and its periodic image at $z = L_z$) in the xy plane. Due to the short range nature of the repulsive monomer wall potential, monomer–monomer interactions across the wall can occur. This can lead to wrong results for the interaction energies and thus, if this contribution is strong enough, for the melt structure near the walls. This is most simply avoided by, e.g., making the simulation box larger by introducing an extra wall at $L_z^{total} = L_z + \delta$, where δ is chosen large enough to prevent

monomer–monomer interactions across the walls. This correction only applies if one uses our method in connection with periodic boundary conditions also in the direction of confinement.

We have checked that all results of film properties shown in Ref. 1 remain the same within error bars. Thus, this correction has no impact on the results and the conclusions presented in Ref. 1.

REFERENCES

- 1 H.-P. Hsu and K. Kremer, *J. Chem. Phys.* **153**, 144902 (2020).
- 2 J. D. Halverson, T. Brandes, O. Lenz, A. Arnold, S. Bevc, V. Starchenko, K. Kremer, T. Stuehn, and D. Reith, *Comput. Phys. Commun.* **184**, 1129 (2013).
- 3 H. V. Guzman, N. Tretyakov, H. Kobayashi, A. C. Fogarty, K. Kreis, J. Krajniak, C. Junghans, K. Kremer, and T. Stuehn, *Comput. Phys. Commun.* **238**, 66 (2019).