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Addition/Correction

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A Systematically Coarse-Grained Solvent-Free Model for Quantitative Phospholipid Bilayer Simulations

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In the Supporting Information of this paper, we provided tables for the pair forces and pair potentials between all coarse grained beads of our lipid model. While the tables for the forces are correct, *the ones for the potential are wrong*. Due to an idiosyncrasy in the way force tables are stored in the ESPResSo package, the integrals over the bare force tables are *not* the potential energies, since the force tables store $F(r)/r$ and not $F(r)$. In this Erratum to our Supporting Information, we provide the correct potential energies ("jp301183m_si_001.zip").

We would like to point out that this error *does not affect any of the results or conclusions of our paper*, in particular not the validity of our model itself. Since the ESPResSo package actually never uses the potential energies when performing a pure molecular dynamics simulation, the incorrect tables were never used (which also explains why we did not instantly notice the problem). However, other molecular dynamics packages use the potentials. For instance, GROMACS reads the potential energy and *from there* creates the force tables by numerical differentiation. Hence, using our old tables for the potential energy and using them in GROMACS leads to incorrect results (in fact, any initially constructed bilayer will fall apart). The new corrected tables ("jp301183m_si_001.zip") resolve this problem.

The only aspect of our original paper that requires a modification is our Figure 7, in which we plot examples of interaction potentials. Their corrected version, contained in this erratum, not only has a slightly different functional form. The most noticeable difference is that the magnitude of the potential energy is bigger.

We are very grateful for Christoph Junghans for pointing out this unfortunate mistake.

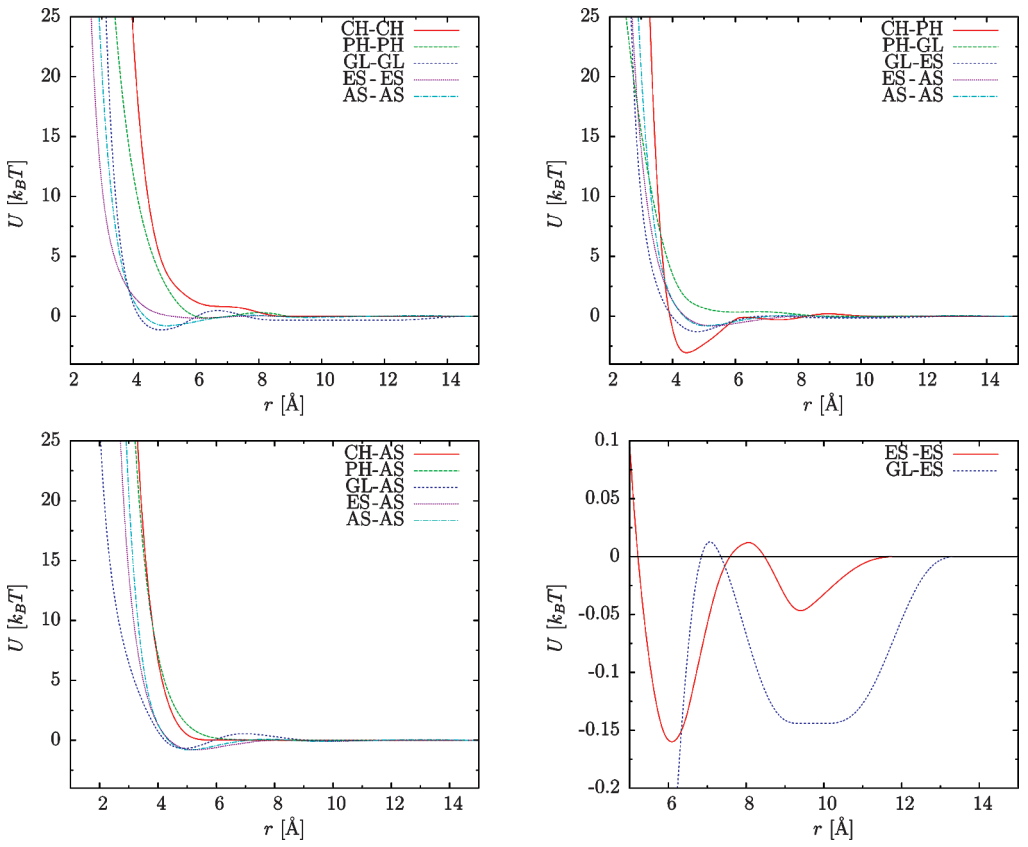

Figure 7. Selected nonbonded interacting potentials between CG beads.

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