Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Transferable potentials for coarse-grained simulations of block copolymer biomimetic membranes[1] MALGORZATA KOWALIK, IAN SINES, JANNA K. MARANAS, MANISH KUMAR, Department of Chemical Engineering, The Pensylvannia State Univeristy, University Park, PA 16802 — We present a framework of minimal model transferable coarse-grained potentials for use in molecular dynamics simulations of amphiphilic block copolymer biomimetic membranes. Testing two, three, and five-bead models of polyethylene oxide polyethylethylene (PEO-PEE) polymer membranes, we show that values for membrane thickness and area per polymer chain obtained using the two-bead model are consistent with our experimental and previously published data. The calculated variation in membrane thickness (d) with hydrophobic molecular weight (M_h) conforms to a known scaling law ($d \sim M_h^a$). The same scaling exponent describes the area per polymer chain. We demonstrate that cross interactions can be represented using combining rules with the use of a scaling factor which is correlated with the difference in hydrophobicities of the interacting hydrophobic/hydrophilic monomers. In this way it becomes possible to rapidly simulate and screen new combinations of block copolymers with minimal potential development effort.

[1]US Department of Energy, Office of Advanced Scientific Computing; grant number DE-FG02-02ER25535

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Date submitted: 11 Nov 2014 Electronic form version 1.4