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Electronic Supplementary Information

Self-assembly of amphiphilic polymers of varying architectures near attractive surfaces

Michiel G. Wessels[1], *and Arthi Jayaraman*[1,2,*]

1. 150 Academy Street, Colburn Laboratory, Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE 19716, USA

2. Department of Materials Science and Engineering, University of Delaware, Newark, DE 19716, USA

***Corresponding author E-mail:** arthij@udel.edu

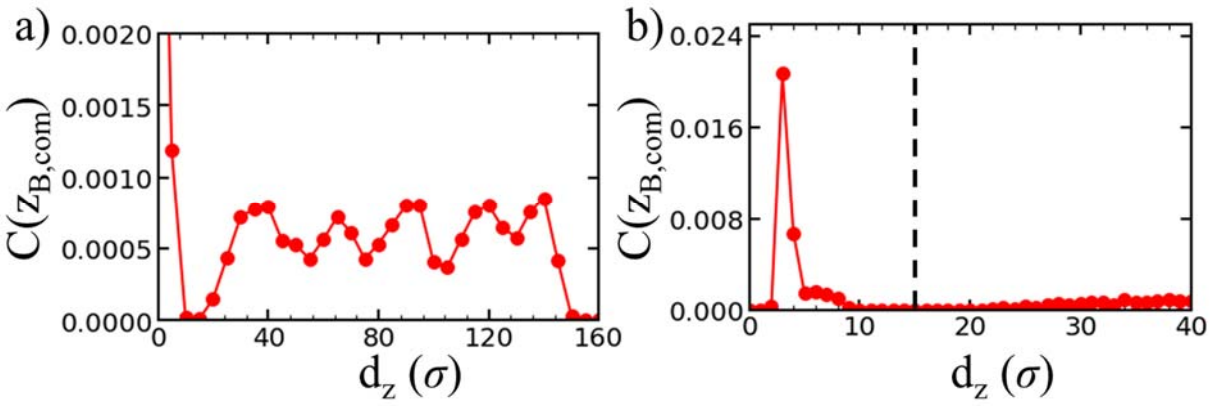

Figure S1. Concentration of center of mass of the B block $C(z_{B,com})$ as a function of distance from the surface (d_z). Part b is a zoomed-in version of part a. The vertical dashed line in part b indicates the cut-off distance below which we consider the chains as being adsorbed to the surface. This data is at ε_{BB}=0.6 for N_{bb}=12 N_{sc}=7 z=4 polymer at η = 0.025, produced with protocol 1 and ε_{WB}=0.4.

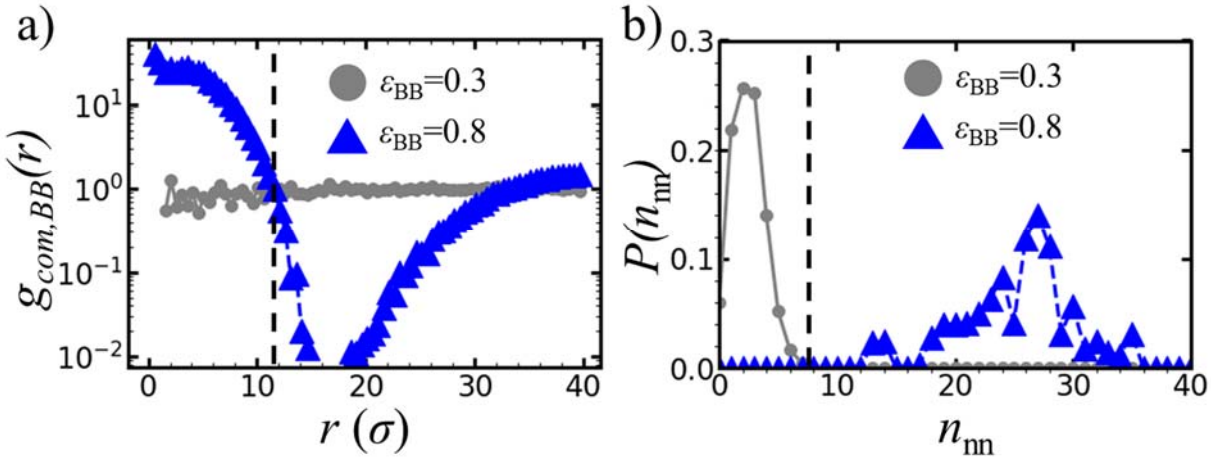

Figure S2. (a) Radial distribution function (RDF) of B-block center of mass at η = 0.025 with no surface. The vertical dashed line in (a) indicates the critical distance where the RDF reaches 1. (b) The neighbor probability distribution within the critical distance shown in part a. The minimum number of nearest neighbors (n_{nn}) to be defined as part of a cluster is shown by the vertical dashed line in part b; this n_{nn} is chosen to identify chains that are not part of clusters (i.e., unimers). This data for N_{bb}=4 N_{sc}=23 z=1 polymer.

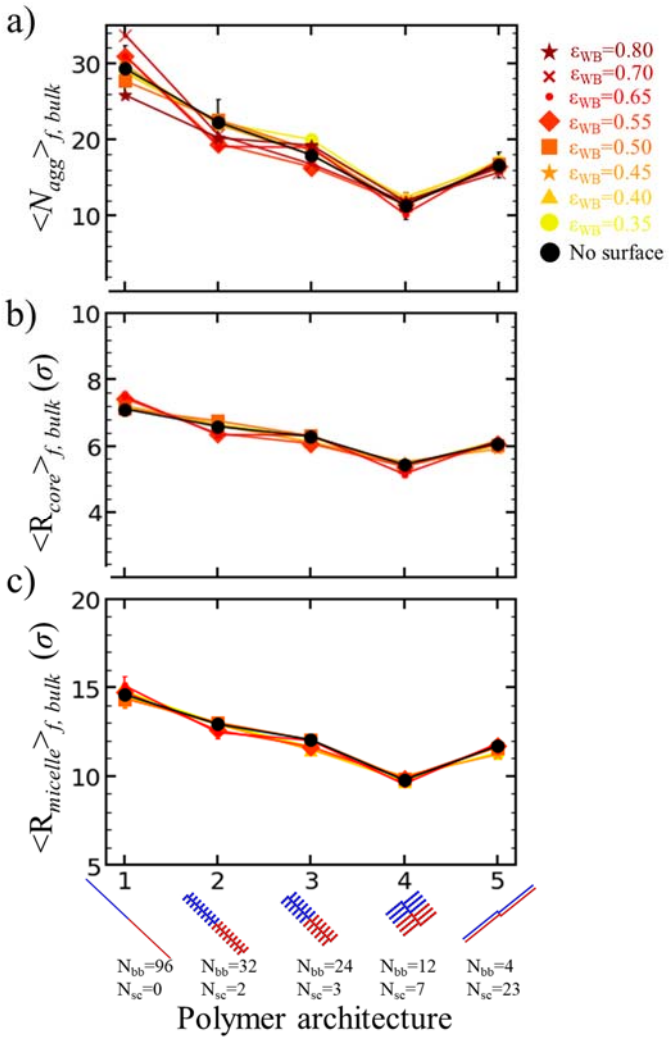

Figure S3. (a) Aggregation numbers, (b) micelle core size, and (c) micelle size for micelles formed away from the surface for polymer architectures with $z = 1$. In this figure, we compare simulations without and with surfaces with varying affinity to B block, as described in the legend.

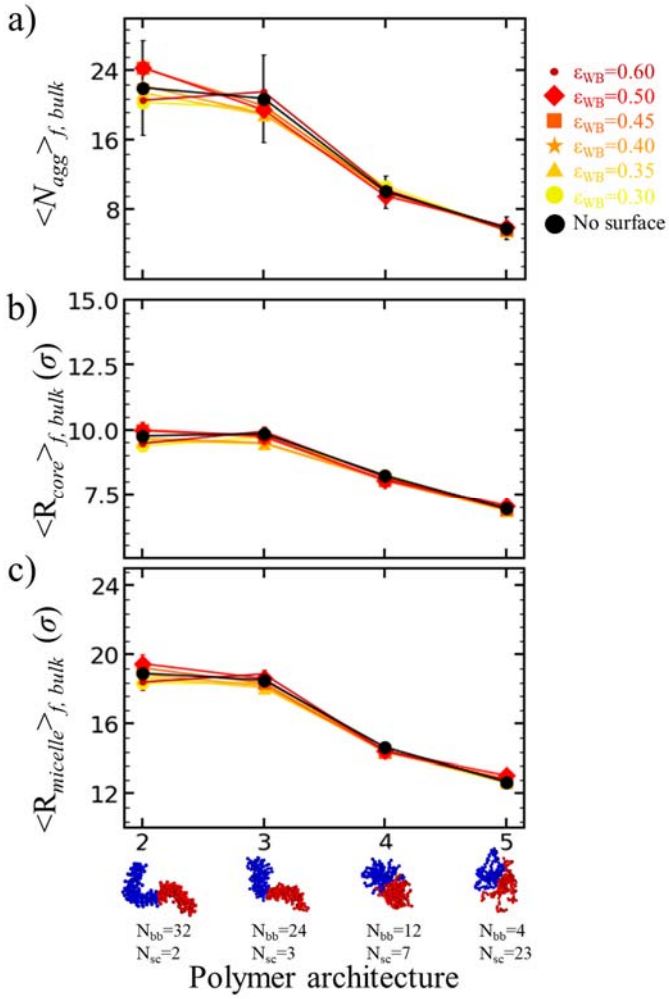

Figure S4. Same as Figure S3 but for $z = 4$.

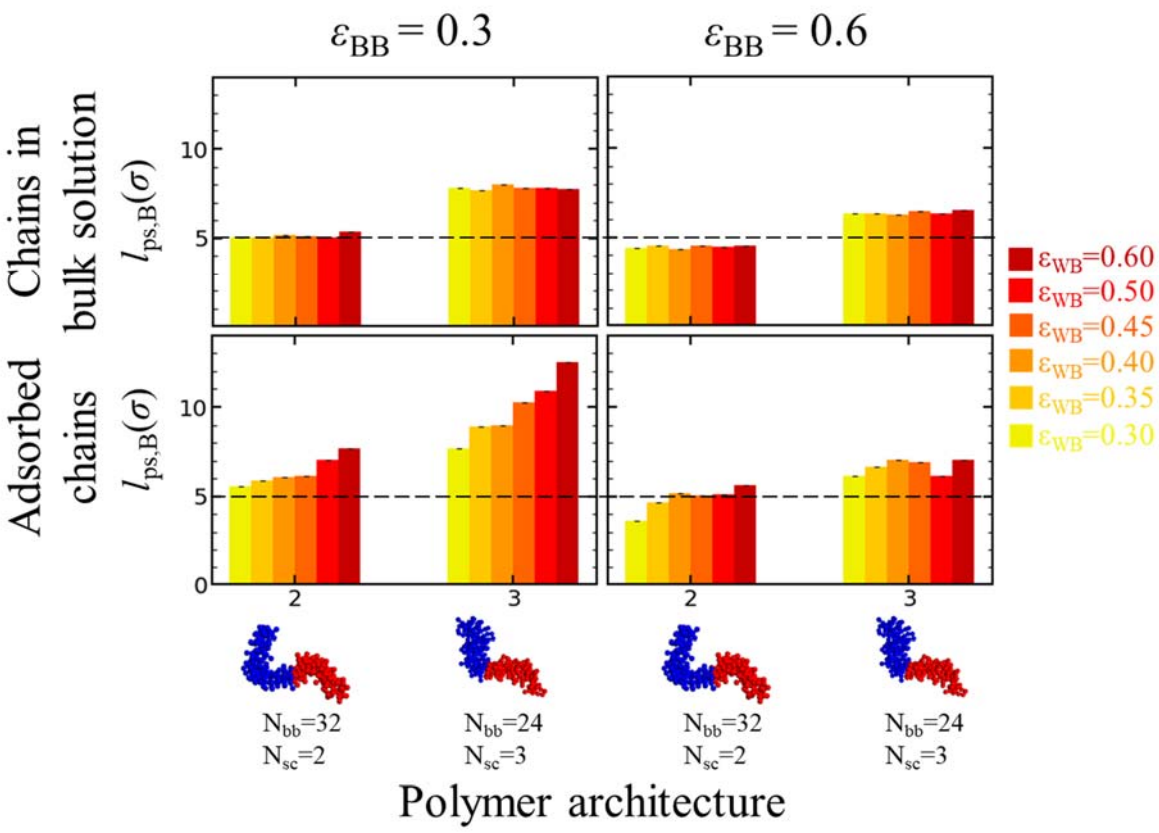

Figure S5. Chain solvophobic B block persistence length, $l_{ps,B}$, for polymer architectures with z = 4 at different fixed values of ε_{WB} and at two values of ε_{BB} as indicated at the top of the figure. The horizontal dashed lines are only to serve as a guide to the eye.

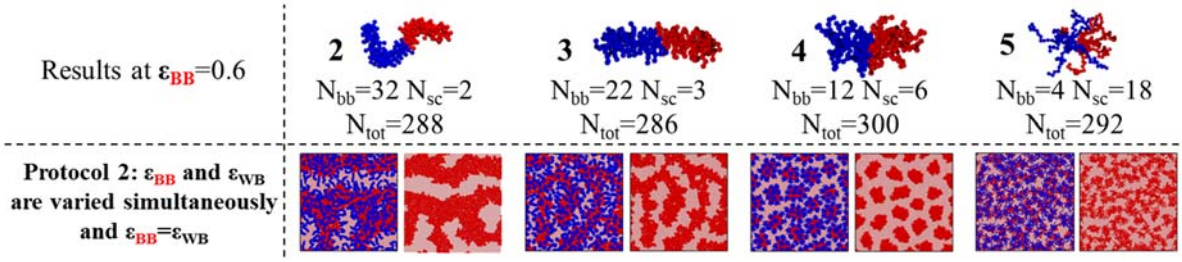

Figure S6. Assembled domains for polymer architectures 2 to 5 with z=4 and **similar** N_{tot} (~295) on solvophobic surfaces with protocol 2 where ε_{WB} and ε_{BB} are kept equal and varied simultaneously. All images shown are for ε_{BB}=0.6. For each architecture, all the beads are shown on the left and the solvophilic beads are hidden on the right to show the solvophobic domains clearly.

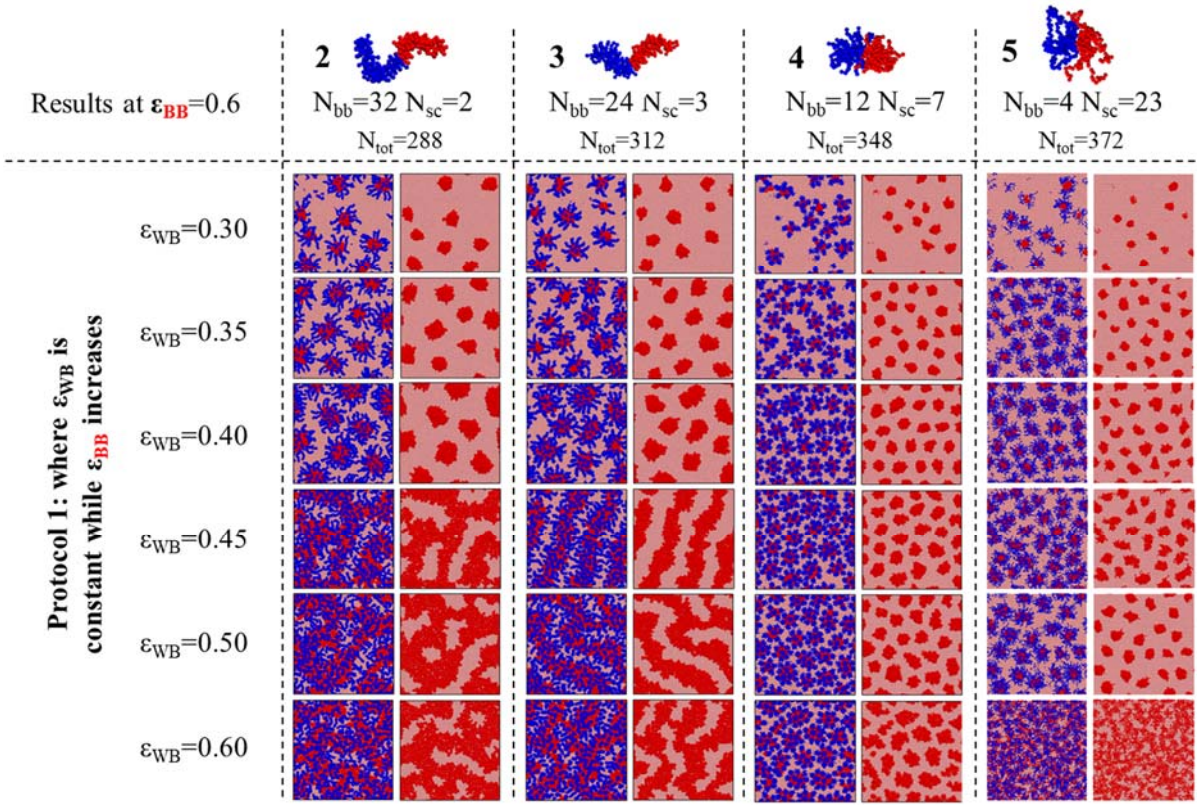

Figure S7. Assembled domains on **hexagonal-packed solvophobic surfaces** for polymer architectures 2 through 5 with z=4 and varying N_{tot} (for architectures 2 through 5 N_{tot}=288, 312, 348, and 372, respectively) on solvophobic surfaces with different fixed values of ε_{WB} (rows) as ε_{BB} is varied (protocol 1). All images shown are for ε_{BB}=0.6. For each architecture, all the beads are shown on the left and the solvophilic beads are hidden on the right to show the solvophobic domains clearly.

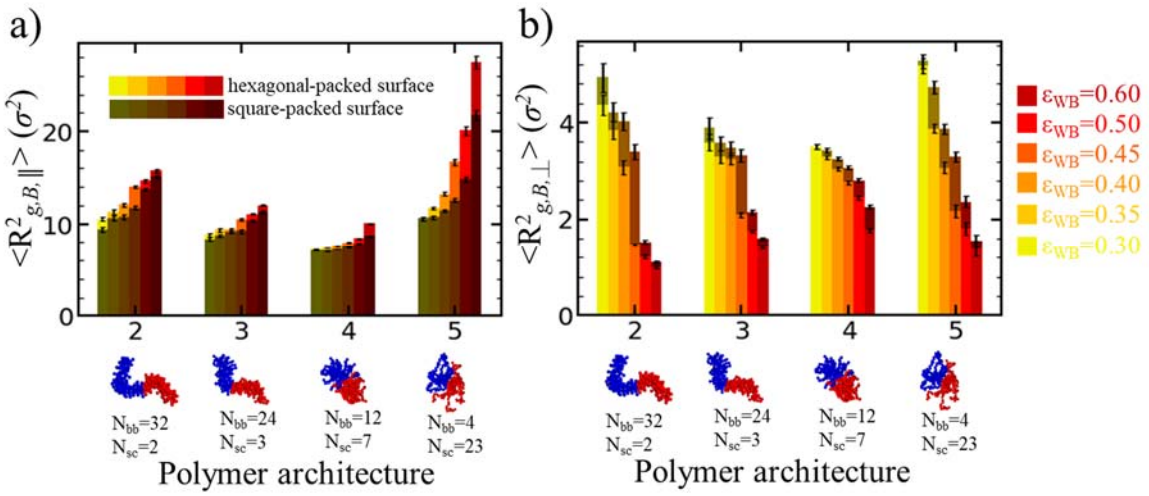

Figure S8. Adsorbed chain structural characteristics on a **hexagonal-packed vs. square-packed surface** for polymer architectures with z = 4 at different fixed values of ε_{WB} with the parallel (a) and perpendicular (b) components of the radius of gyration of the solvophobic block at ε_{BB} = 0.6.

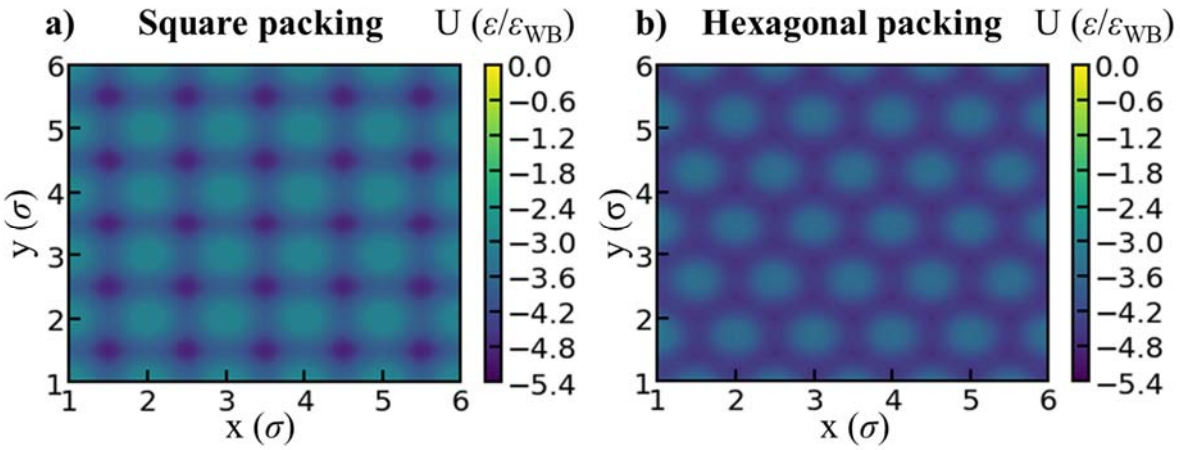

Figure S9. The Lennard-Jones interaction potential energies faced by a solvophobic bead with ε_{WB}=1 across surfaces with (a) square-packed and (b) hexagonal-packed two-dimensional lattices.