

Supplementary information to

**Nanotribology of biopolymer brushes in aqueous solution using
dissipative particle dynamics simulations: an application to PEG covered
liposomes in theta solvent**

A. Gama Goicochea¹¹, E. Mayoral¹, J. Klapp^{1,2}, and C. Pastorino³

¹Instituto Nacional de Investigaciones Nucleares, Carretera México – Toluca s/n, La
Marquesa Ocoyoacac, Estado de México 52750, Mexico

²Departamento de Matemáticas, CINVESTAV del IPN, México D. F. 07360, Mexico

³Departamento de Física, Centro Atómico Constituyentes, CNEA – CONICET, Av.
General Paz 1499, Provincia de Buenos Aires 1650, Argentina

¹ Corresponding author. Electronic mail: agama@alumni.stanford.edu

Supplementary information

In here we provide the data used for the graphs shown in Figure 8(a) and 8(b) of the manuscript entitled “Nanotribology of biopolymer brushes in aqueous solution using dissipative particle dynamics simulations: an application to PEG covered liposomes in theta solvent”, see reference [S1].

In Table SI, the first, third and fifth columns correspond to the values of the shear rate applied to the surfaces onto which polymer chains were grafted for the cases when the polymerization degrees were equal to $N=7$, $N=14$, and $N=20$ and $N=25$, respectively. The values for the shear rate on the fifth column were applied to both the $N=20$ and $N=25$ cases.

For the calculation of the friction coefficient we used the equation $\mu = \langle F_x(\dot{\gamma}) \rangle / \langle F_z(\dot{\gamma}) \rangle$, see, for example, reference [S2], where $F_x(\dot{\gamma})$ represents the magnitude of the force on the particles grafted onto each surface along the direction of the shear rate, $\dot{\gamma}$, and $F_z(\dot{\gamma})$ is the magnitude of the force on the particles, acting perpendicularly to the surfaces. The brackets indicate the time average of the forces over the positions of the particles obtained at each time step.

TABLE SI

$\dot{\gamma}$	$\mu(N=7)$	$\dot{\gamma}$	$\mu(N=14)$	$\dot{\gamma}$	$\mu(N=20)$	$\mu(N=25)$
2.86×10^{-4}	1.03×10^{-4}	2.86×10^{-4}	3.77×10^{-4}	2.86×10^{-4}	9.41×10^{-4}	0.00176379
5.71×10^{-4}	2.00×10^{-4}	5.71×10^{-4}	6.42×10^{-4}	5.71×10^{-4}	0.00170046	0.00288892
8.57×10^{-4}	2.01×10^{-4}	8.57×10^{-4}	0.0010901	8.57×10^{-4}	0.00247495	0.00534289
0.00285714	8.14×10^{-4}	0.00143	0.00173534	0.00114286	0.00361833	0.00590847
0.00571429	0.00173179	0.00229	0.00272533	0.00142857	0.00533876	0.00794264
0.00857143	0.00242778	0.00286	0.00314444	0.00171429	0.00596622	0.00984506
0.01142857	0.00321594	0.00571	0.00654071	0.00228571	0.00746346	0.01168807
0.01428571	0.00410414	0.00857	0.00960247	0.00285714	0.00960085	0.01457752
0.01714286	0.0046823	0.01143	0.01245625	0.00571429	0.01633275	0.0228637
0.02	0.00573045	0.01429	0.01491178	0.00857143	0.02191747	0.03071073
0.02285714	0.0065128	0.01714	0.01773832	0.01142857	0.0268266	0.03583409
0.02571429	0.00730424	0.02	0.02003882	0.01428571	0.03071406	0.04114384
0.02857143	0.00800893	0.02286	0.02251486	0.01714286	0.03511389	0.04586099
0.05714286	0.01585463	0.02571	0.02451455	0.02	0.03906288	0.05043854
0.08571429	0.02341354	0.02857	0.02670734	0.02285714	0.04219836	0.05507711

TABLE SI (continued)

$\dot{\gamma}$	$\mu(N=7)$	$\dot{\gamma}$	$\mu(N=14)$	$\dot{\gamma}$	$\mu(N=20)$	$\mu(N=25)$
0.11428571	0.03046697	0.05714	0.0440131	0.02571429	0.04624591	0.05935909
0.14285714	0.0370556	0.11429	0.06903552	0.02857143	0.04972951	0.06358752
0.17142857	0.04364203	0.17143	0.08954294	0.05714286	0.07981672	0.10205479
0.2	0.04994345	0.22857	0.10749842	0.08571429	0.1055679	0.13373305
0.22857143	0.0558129	0.28571	0.12497878	0.11428571	0.128748	0.16306103
0.25714286	0.06150716	-----	-----	0.14285714	0.1508766	0.1903674
0.28571429	0.06715919	-----	-----	0.17142857	0.17080467	0.21656203
-----	-----	-----	-----	0.2	0.19110141	0.24229849
-----	-----	-----	-----	0.22857143	0.20972285	0.26466933
-----	-----	-----	-----	0.25714286	0.22786315	0.28797785
-----	-----	-----	-----	0.28571429	0.2483624	0.31212635

References

[S1] Manuscript “*Nanotribology of biopolymer brushes in aqueous solution using dissipative particle dynamics simulations: an application to PEG covered liposomes in theta solvent*”, A. Gama Goicochea, E. Mayoral, J. Klapp, and C. Pastorino.

[S2] W. C. Makosco. *Rheology. Principles, Measurements and Applications*. Wiley-VCH. New York. 1994.