

Supporting Information

Effects of Concentration and Ionization Degree of Anchoring Cationic Polymers on Lateral Heterogeneity of Anionic Lipid Monolayers

Xiaozheng Duan,¹ Yang Zhang,² Liangyi Li,¹ Ran Zhang,¹ Mingming Ding,^{*,1} Qingrong Huang,³ Wen-Sheng Xu,^{*,4,†} Tongfei Shi^{*,1} and Lijia An¹

¹ State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, 130022, P. R. China

² Northeast Normal University, Changchun, 130024, P. R. China

³ Department of Food Science, Rutgers University, 65 Dudley Road, New Brunswick, New Jersey 08901, USA

⁴ James Franck Institute, The University of Chicago, Chicago, Illinois 60637, United States

* To whom correspondence should be addressed. Email: mmding@ciac.ac.cn, tfshi@ciac.ac.cn, wsxu0312@gmail.com.

† Current address: Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831, United States

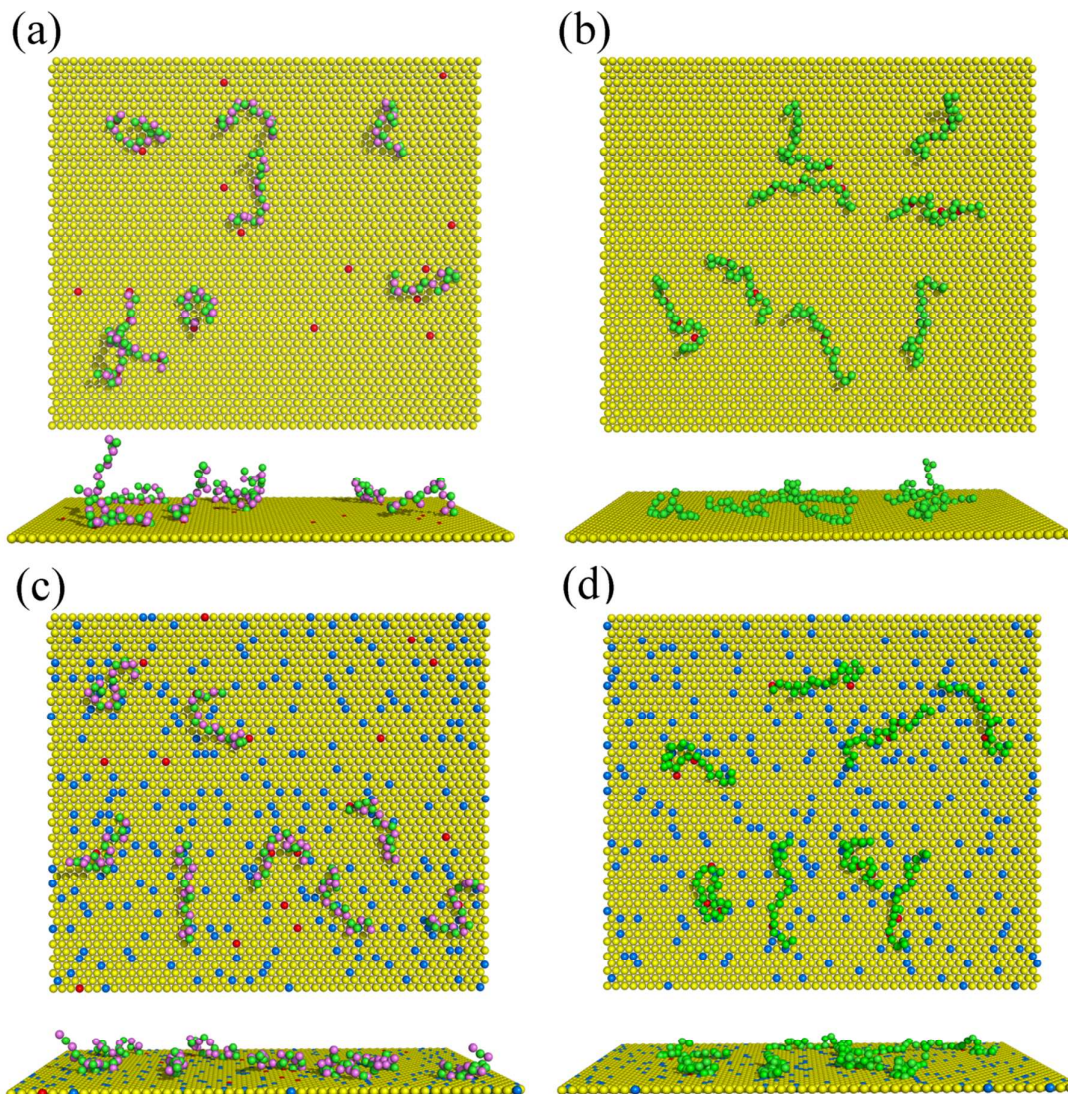


Figure S1. Equilibrated configurations of the polymers/monolayer complexes for the case of $C_p=0.00185$. The results are for (a, b) PC:PIP₂=99:1 and (c, d) PC:PS:PIP₂=89:10:1. Green and violet spheres denote the cationic and charge-neutral segments of the polymers; red, blue and yellow spheres represent the PIP₂, PS and PS lipid headgroups. The segmental ionizations (f) of the polymers are set as (a, c) 0.5 and (b, d) 1.0, respectively.

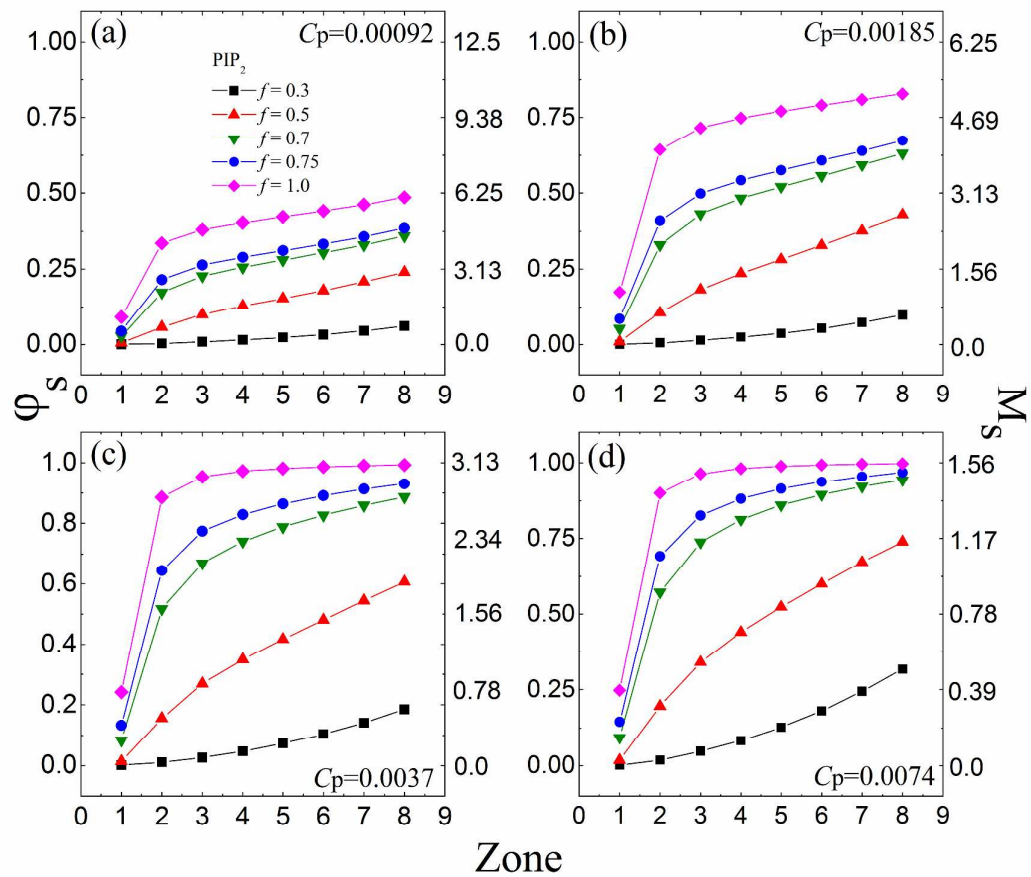


Figure S2. Fraction (ϕ_s) of the total sequestered PIP₂ (solid symbols) and PS (vacant symbols) lipids in the interaction zones of all anchored polymers, and the number (M_s) of PIP₂ (solid symbols) and PS (vacant symbols) sequestered in the interaction zones of each anchored polymer. The segmental ionization fraction (f) varies from 0.3 to 1.0. The polymer concentration ranges from (a) $C_p=0.00092$, (b) $C_p=0.00185$, (c) $C_p=0.0037$ to (d) $C_p=0.0074$. The results shown are for PC:PIP₂=99:1.

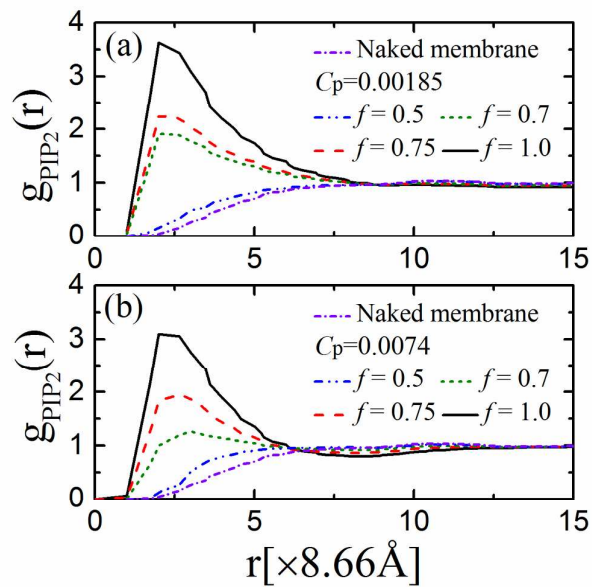


Figure S3. Radial distribution functions of the PIP₂ lipids. The segmental ionization fraction (f) varies from 0.5 to 1.0, and the polymer concentration ranges from $C_p=0.00185$ to $C_p=0.0074$. The results shown are for PC:PIP₂=99:1.

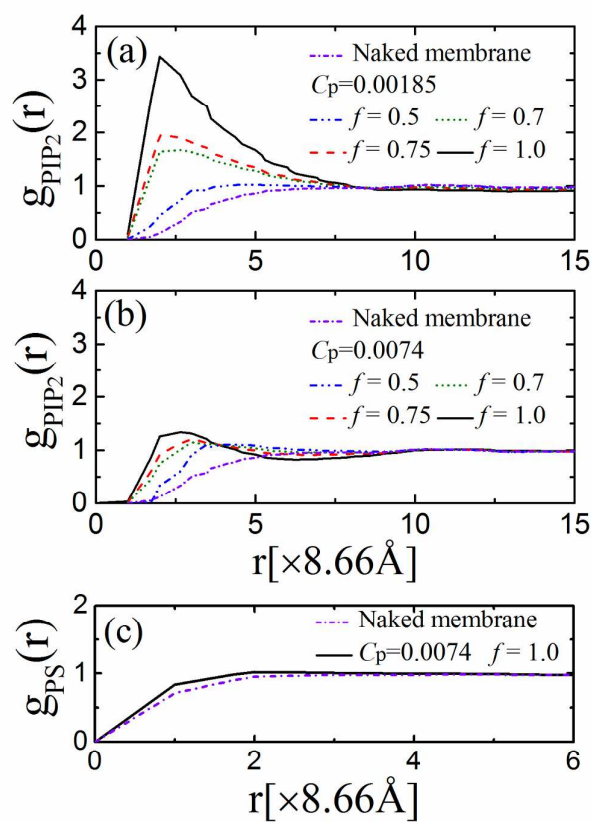


Figure S4. Radial distribution functions of the PIP_2 and PS lipids. The segmental ionization fraction (f) varies from 0.5 to 1.0, and the polymer concentration ranges from $C_p=0.00185$ to $C_p=0.0074$. The results shown are for PC:PS: PIP_2 =89:10:1.

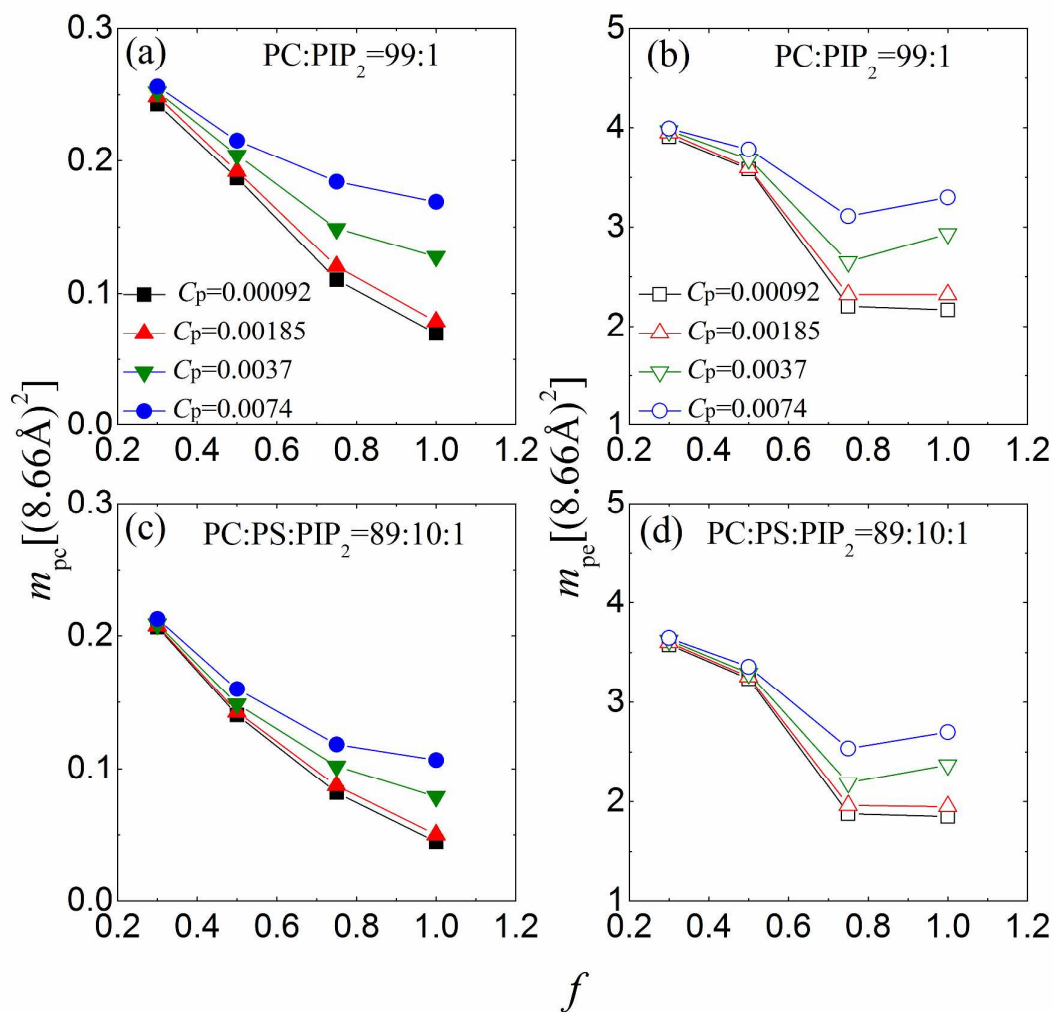


Figure S5. MSD of (a, c) the center of mass (m_{pc}) and (b, d) the ends (m_{pe}) of the anchored polymers in each 50 MC steps. The segmental ionization fraction (f) varies from 0.3 to 1.0, and the polymer concentration (C_p) ranges from $C_p=0.00092$ to $C_p=0.0074$. The results shown are for (a, b) PC:PIP₂=99:1 and (c and d) PC:PS:PIP₂=89:10:1.

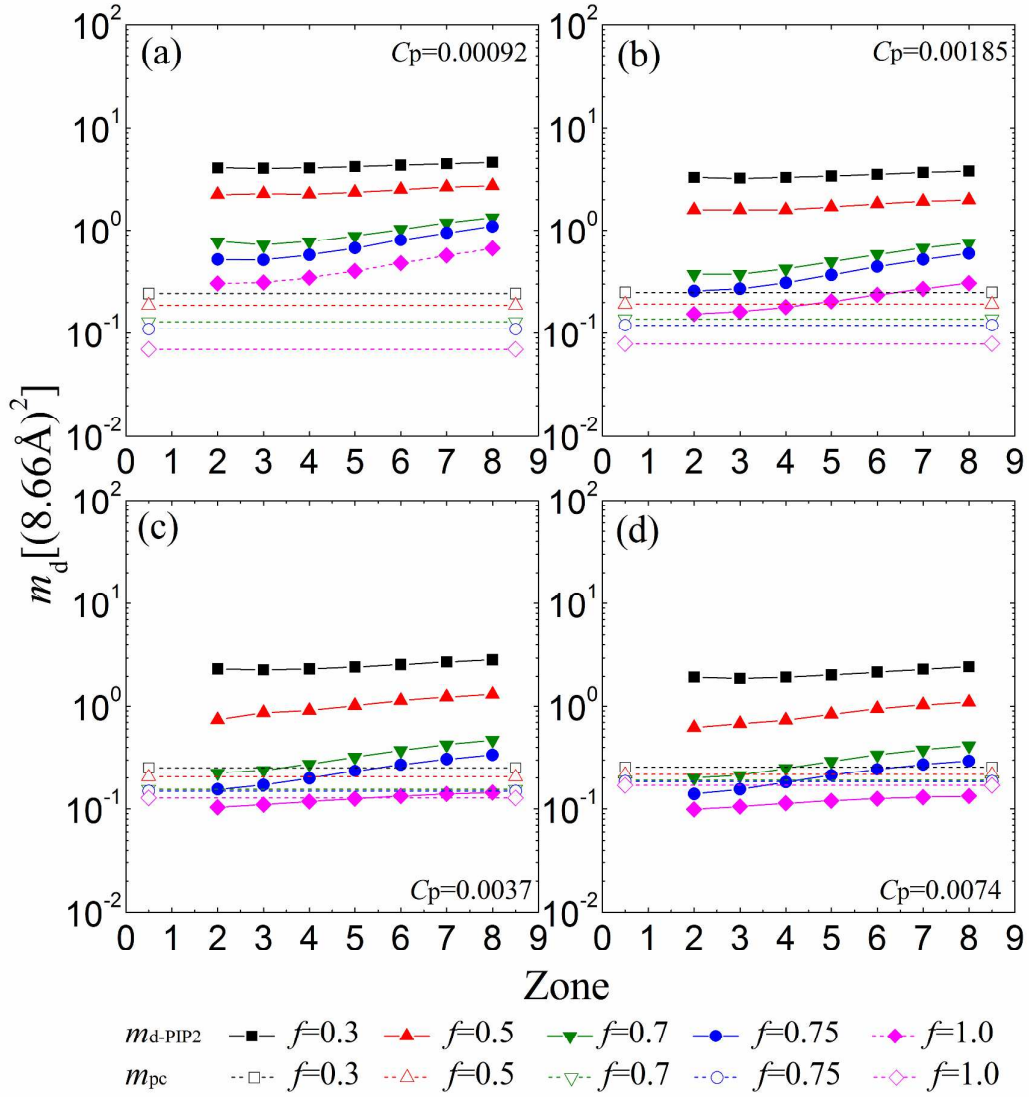


Figure S6. MSD of the center of mass of the sequestered PIP₂ micro-domains (m_{d-PIP_2} , the solid symbols and solid lines), and MSD of the center of mass of the anchored polymers (m_{pc} , the vacant symbols and dashed lines) in each 50 MC steps. The segmental ionization fraction (f) varies from 0.3 to 1.0, and the polymer concentration (C_p) ranges from (a) $C_p=0.00092$, (b) $C_p=0.00185$, (c) $C_p=0.0037$ to (d) $C_p=0.0074$. The results shown are for PC:PIP₂=99:1.

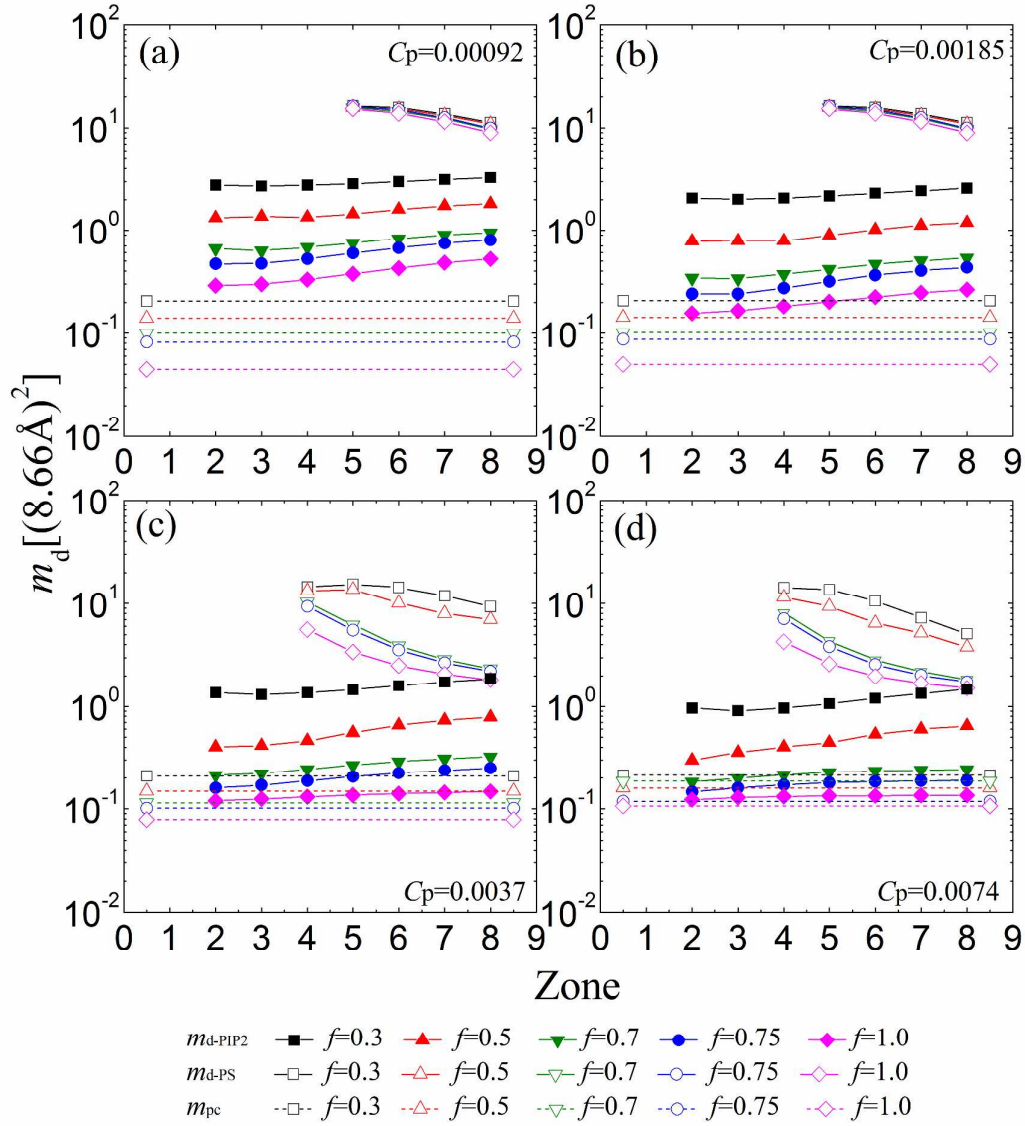


Figure S7. MSD of the center of mass of the sequestered PIP₂ micro-domains (m_{d-PIP_2} , the solid symbols and solid lines) and PS micro-domains (m_{d-PS} , the vacant symbols and solid lines), and MSD of the center of mass of the anchored polymers (m_{pc} , the vacant symbols and dashed lines) in each 50 MC steps. The segmental ionization fraction (f) varies from 0.3 to 1.0, and the polymer concentration (C_p) ranges from (a) $C_p=0.00092$, (b) $C_p=0.00185$, (c) $C_p=0.0037$ to (d) $C_p=0.0074$. The results shown are for PC:PS:PIP₂=89:10:1.

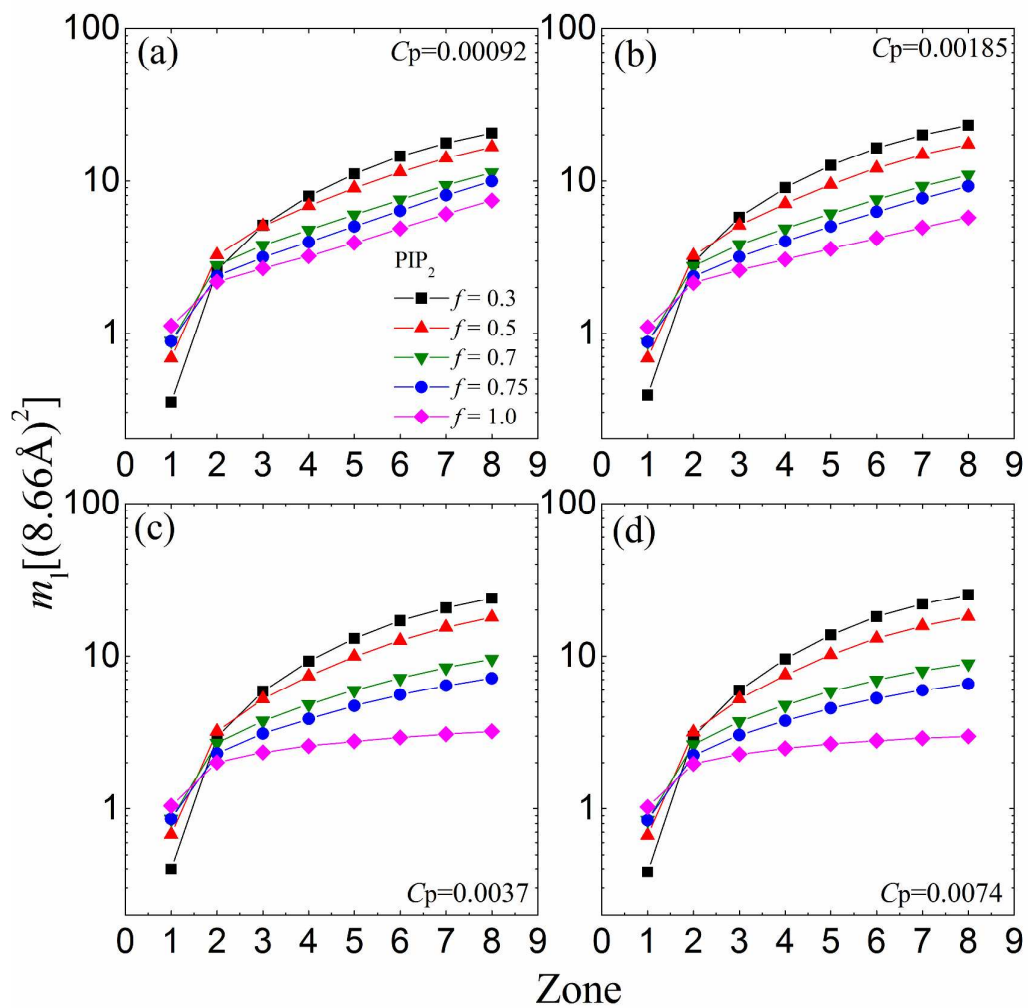


Figure S8. MSD of single PIP₂ (m_{l-PIP_2} , solid symbols and solid lines) sequestered in each interaction zone in each 50 MC steps. The segmental ionization fraction (f) varies from 0.3 to 1.0, and the polymer concentration (C_p) ranges from (a) $C_p=0.00092$, (b) $C_p=0.00185$, (c) $C_p=0.0037$ to (d) $C_p=0.0074$. The results shown are for PC:PIP₂=99:1.

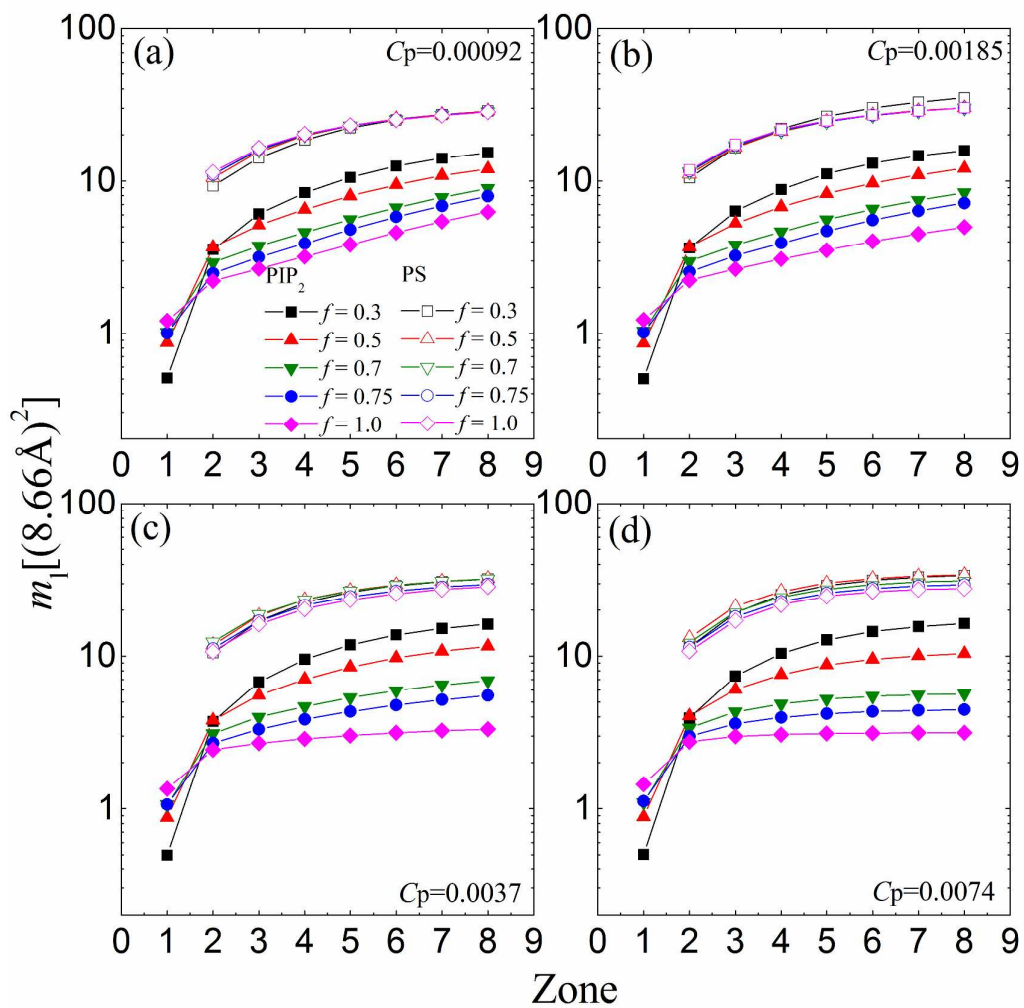


Figure S9. MSD of single PIP₂ (m_{l-PIP_2} , solid symbols and solid lines) and single PS (m_{l-PS} , vacant symbols and solid lines) sequestered in each interaction zone in each 50 MC steps. The segmental ionization fraction (f) varies from 0.3 to 1.0, and the polymer concentration (C_p) ranges from (a) $C_p=0.00092$, (b) $C_p=0.00185$, (c) $C_p=0.0037$ to (d) $C_p=0.0074$. The results shown are for PC:PS:PIP₂=89:10:1.