

Supporting Information

De-swelling mechanisms of surface-grafted poly(NIPAAm) brushes: Molecular dynamics simulation approach

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Figure 1S. Packing energies of the surface-grafted P(NIPAAm) brush.

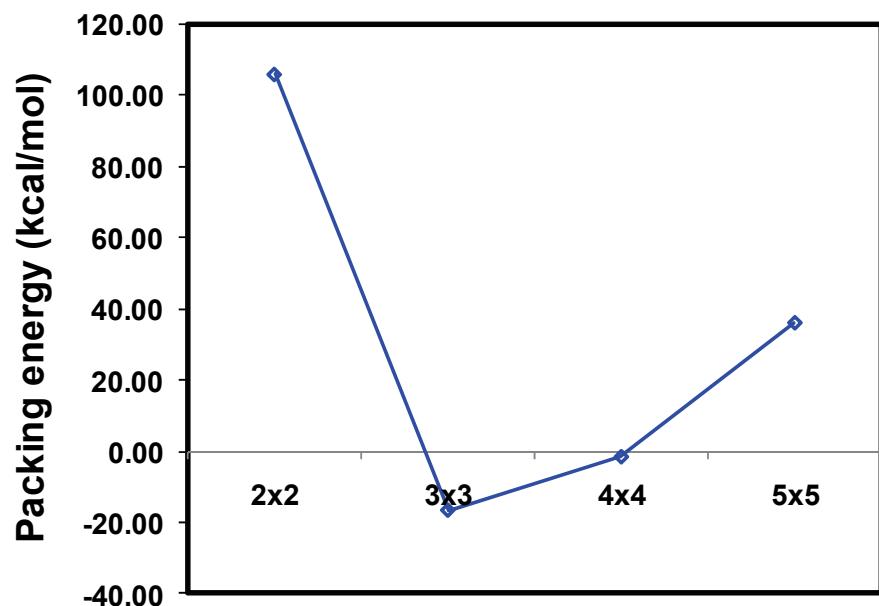
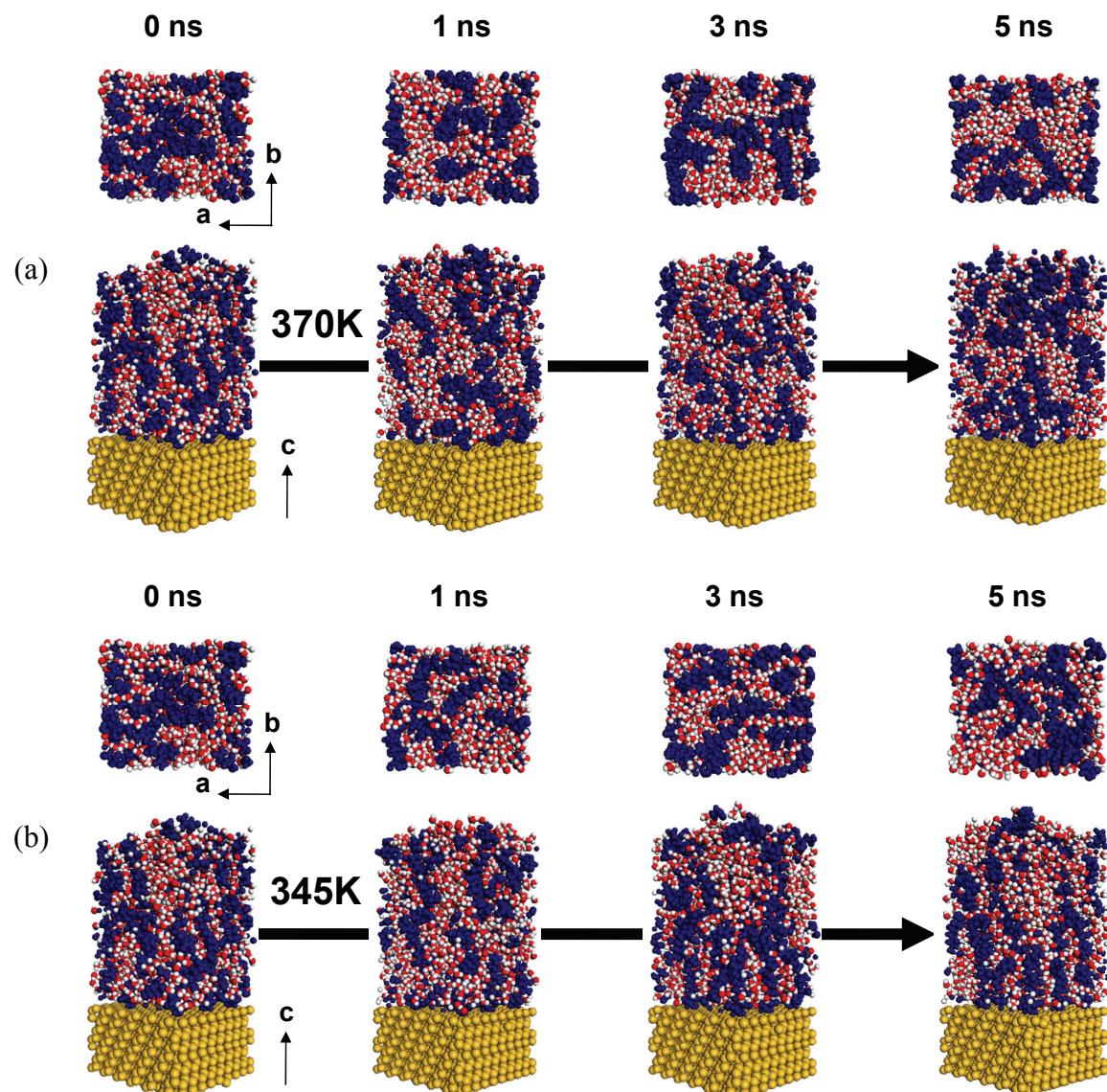
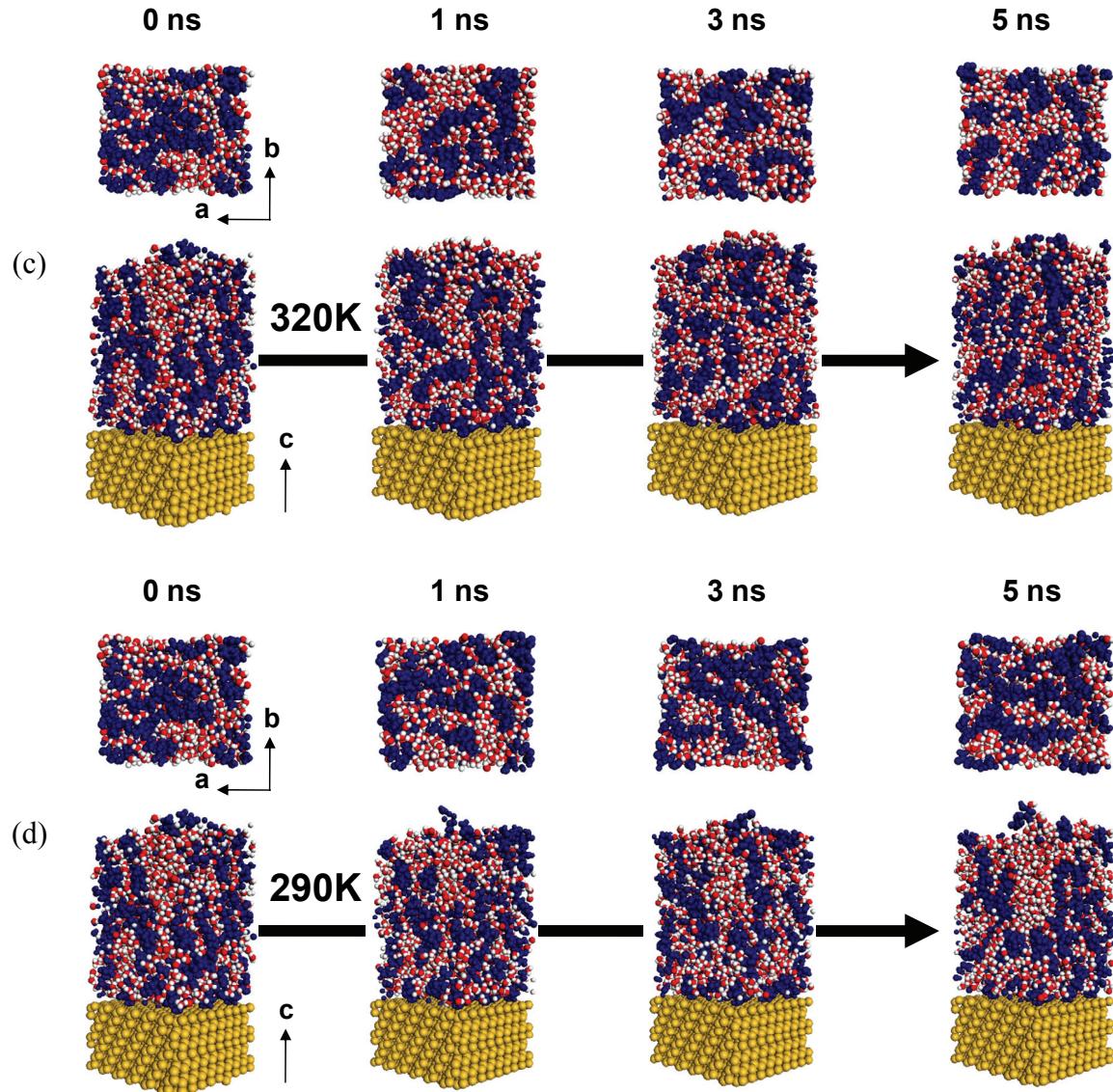


Figure 2S. Snapshots of the hydrated surface-grafted P(AAm) brushes during simulation at (a) 370 K; (b) 345 K; (c) 320 K; (d) 290 K; and (e) 275 K. Blue, yellow, red, and white color denote polymer brushes, silicon substrate, oxygen of water, and hydrogen of water, respectively.





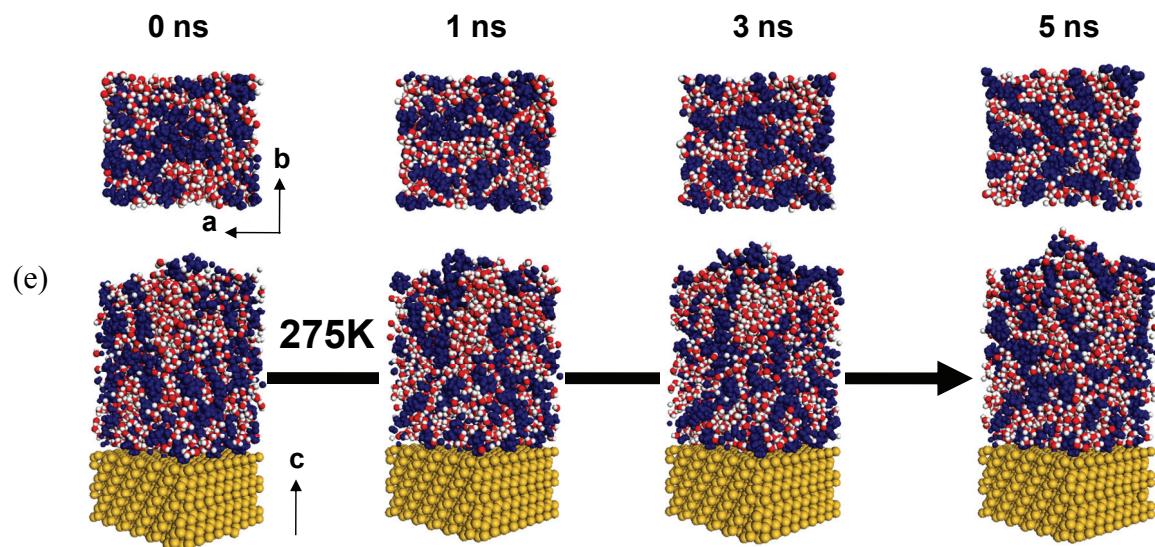
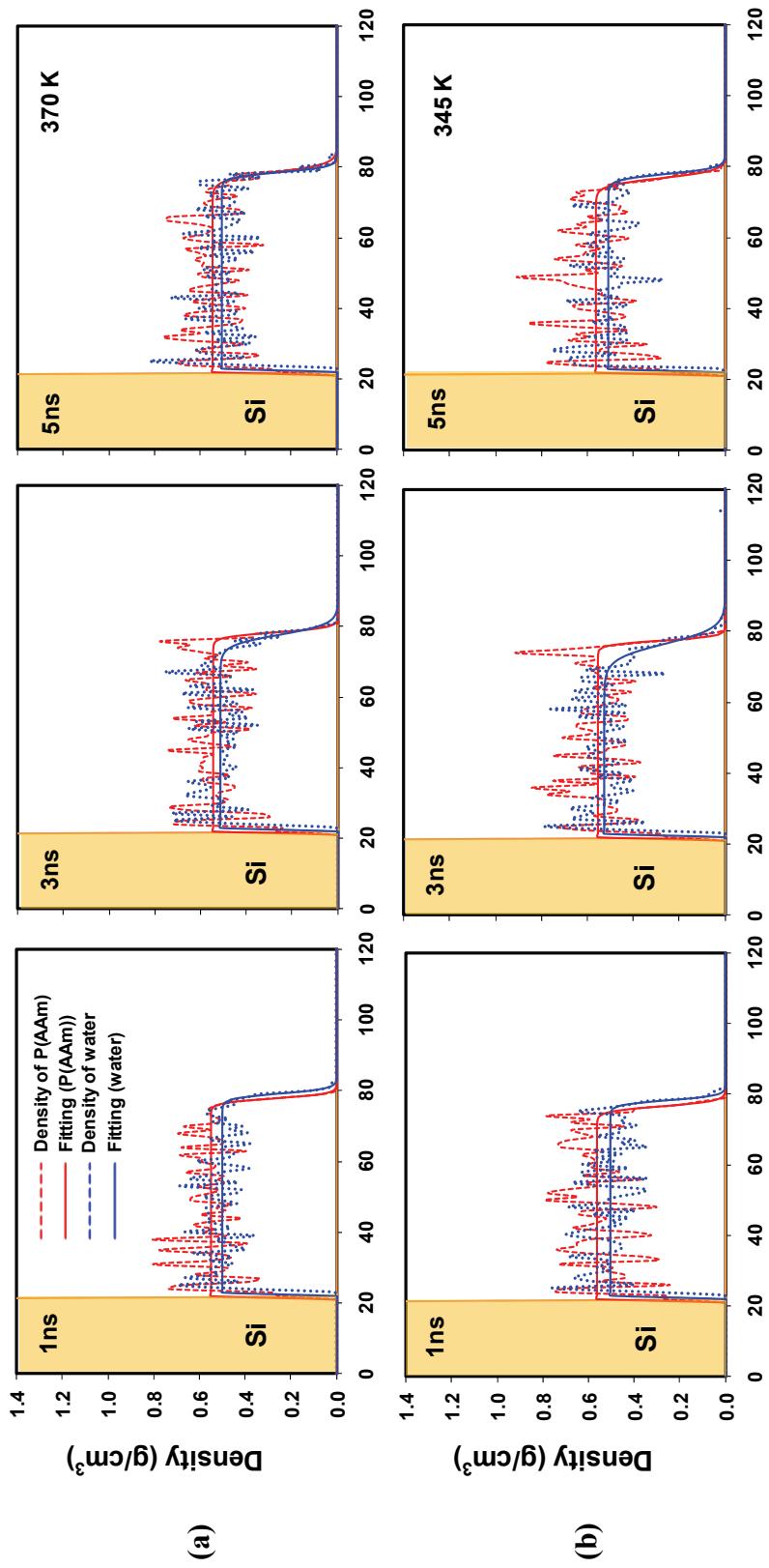


Figure 3S. Density profiles of the surface-grafted P(AAm) brushes at: (a) 370 K; (b) 345 K; (c) 320 K; (d) 295 K; and (e) 275 K.



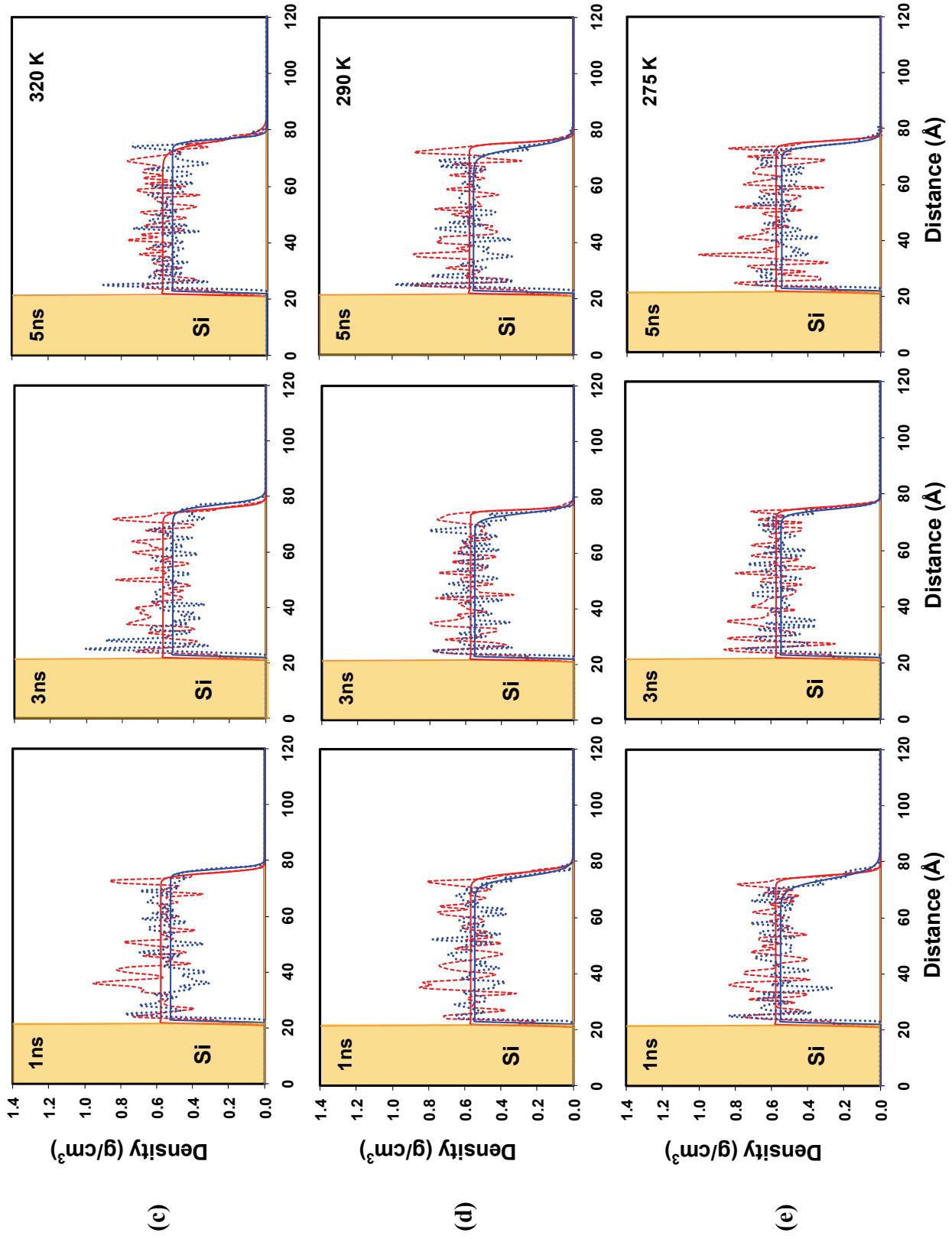


Figure 4S. Thickness of the P(AAm) brushes.

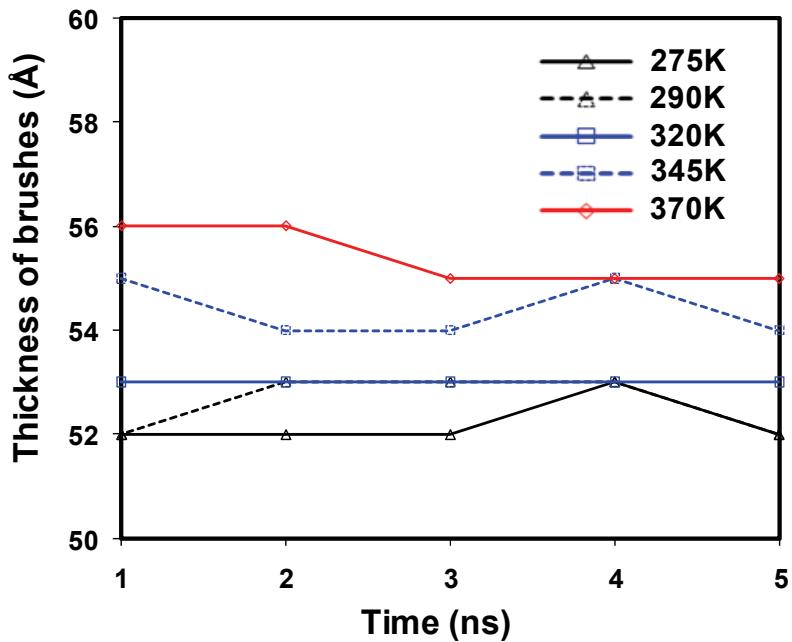


Figure 5S. Pair correlation functions of: (a) O(AAm)-O(water) pairs; and (b) N(AAm)-O(water) pairs.

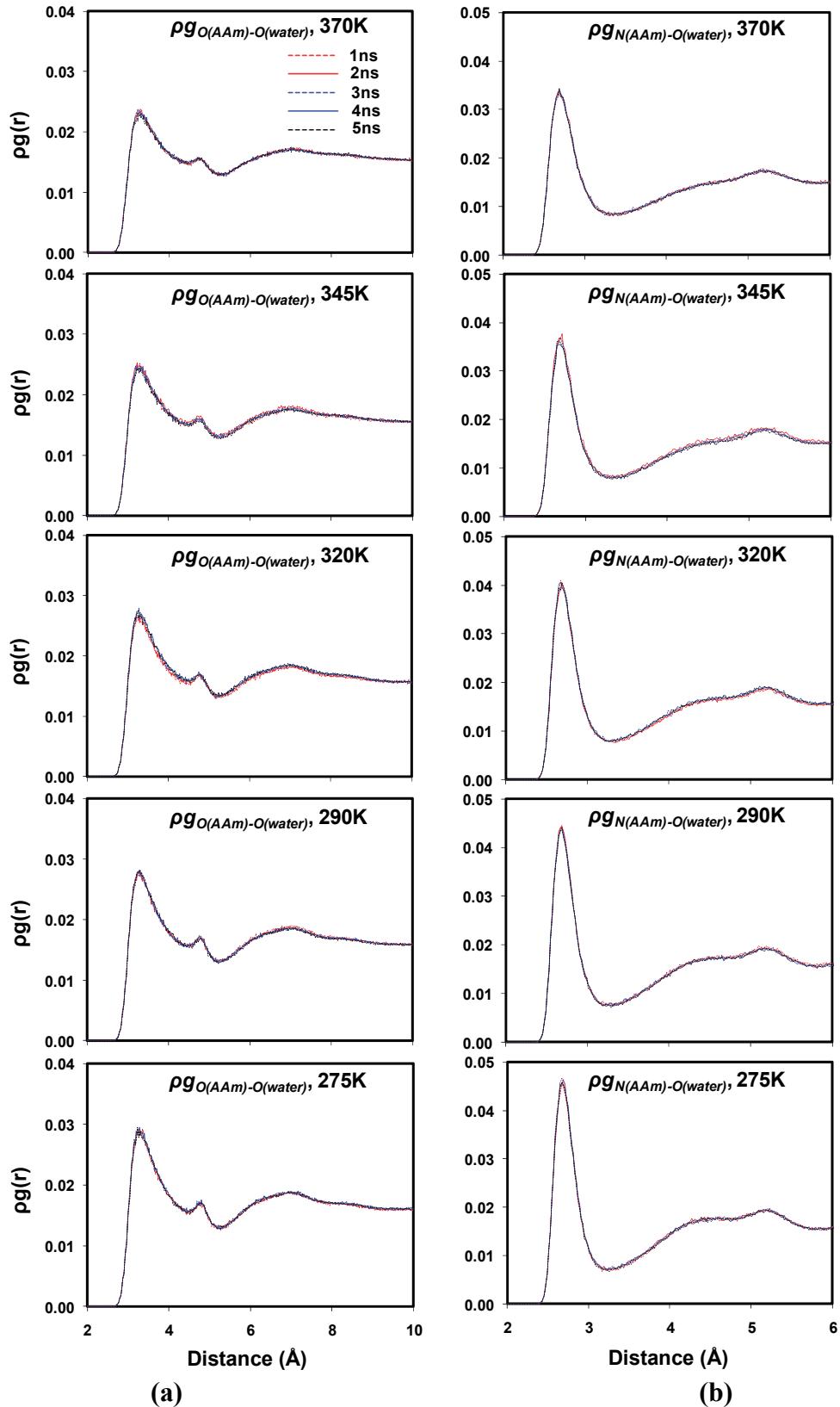


Figure 6S. Change in the coordination numbers of: (a) O(AAm)-O(water) pairs; and (b) N(AAm)-O(water) pairs.

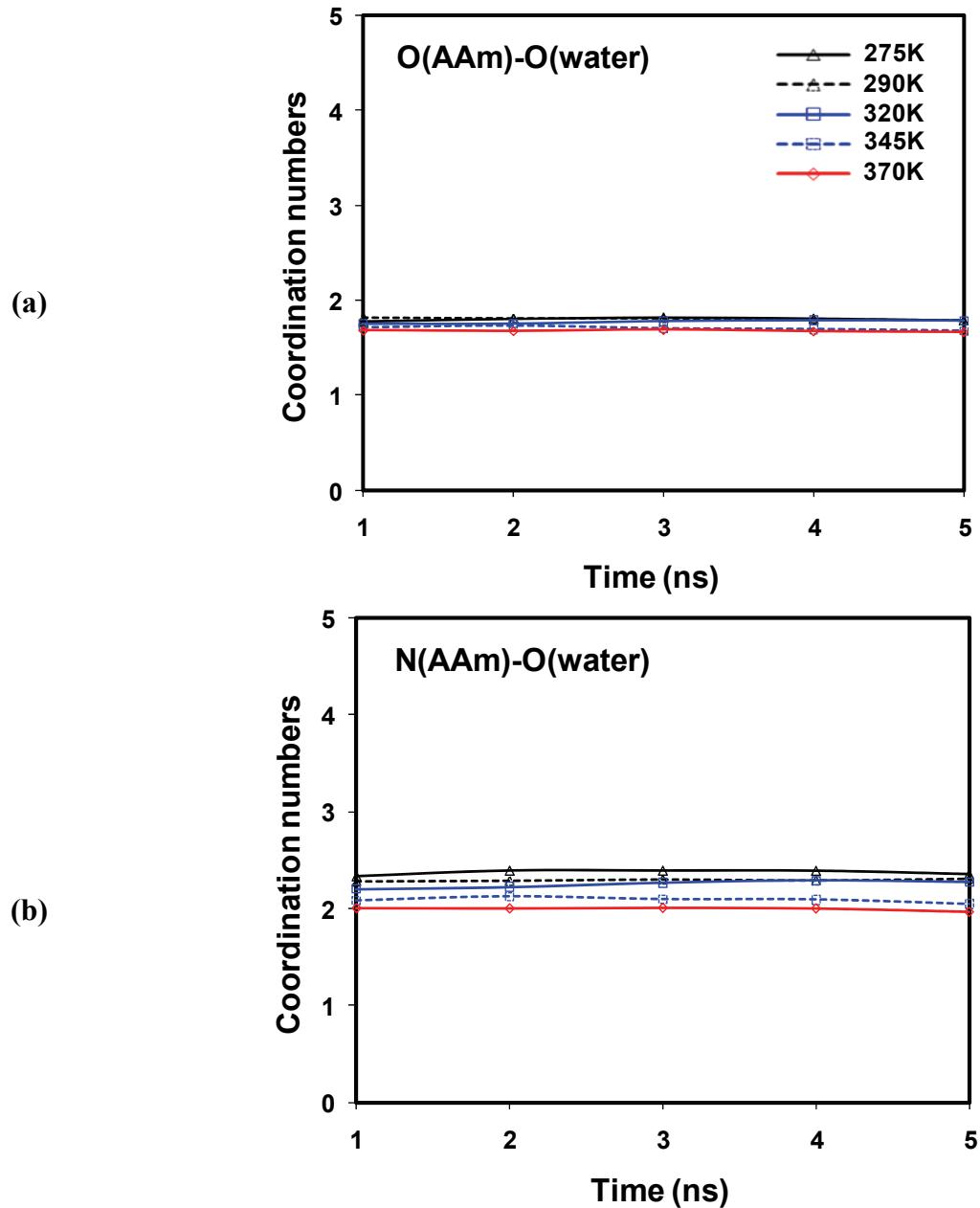


Figure 7S. Total number of hydrogen bonds in P(AAm) brushes.

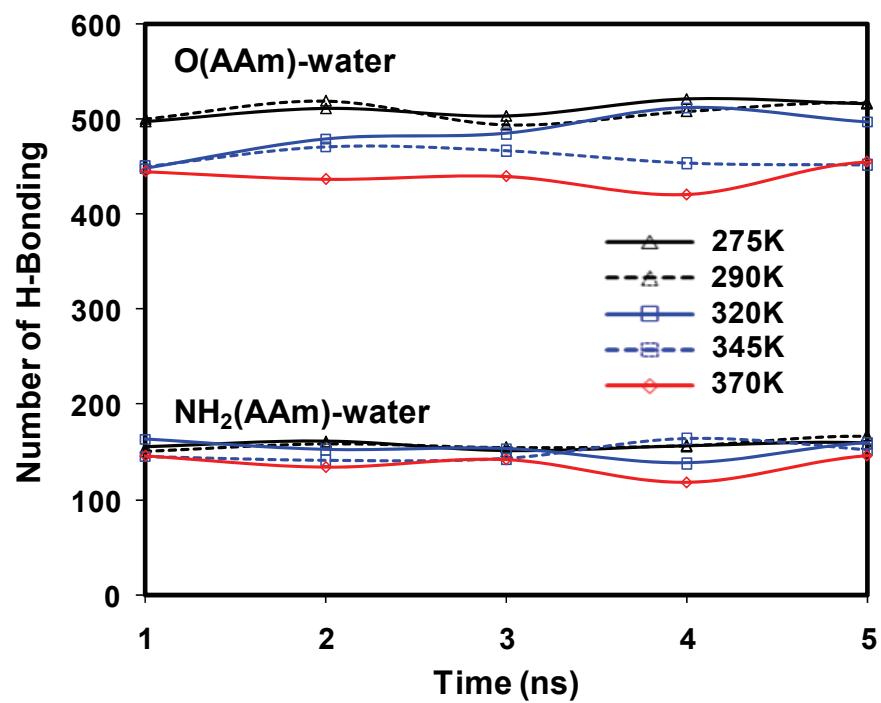


Figure 8S. Total surface area of P(AAm) brushes.

