Electronic Supporting Information

Molecular Investigation of Wettability of Rough Surfaces by Molecular Dynamics Simulation

Hamzeh Yaghoubi, Masumeh Foroutan*

Department of Physical Chemistry, School of Chemistry, College of Science, University of Tehran, Tehran, Iran

*Corresponding author. foroutan@khayam.ut.ac.ir, Tel +98 21 61112896; Fax: +98 21 66495291.

Figure S1 shows the value of $(U_{(\lambda_{i+1})} - U_{(\lambda_i)})$ during the solid-liquid separation for different systems.

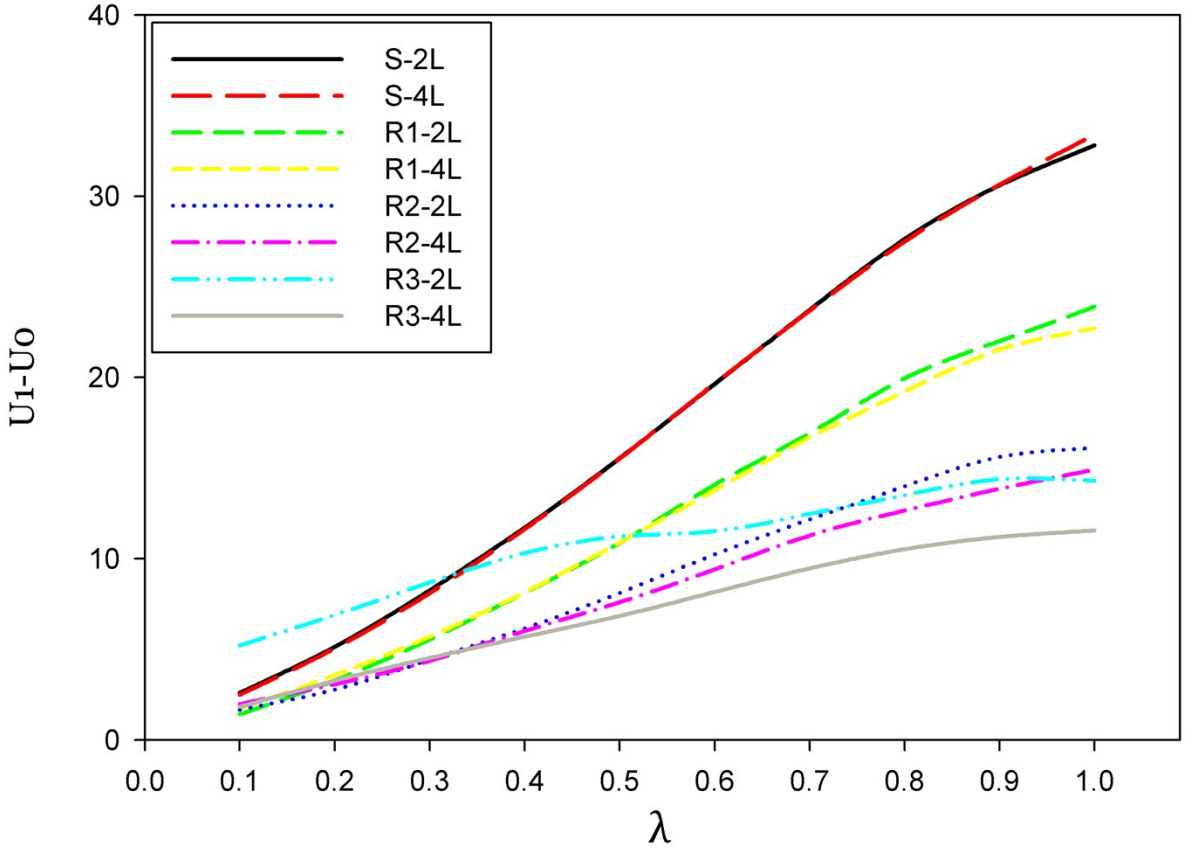

Figure S1. Variation of $(U_{(\lambda_{i+1})} - U_{(\lambda_i)})$ during the solid-liquid separation for different systems.

Figure S2 shows the curves of the PMF versus time during the water removal from substrate surface for different systems. The red circle in each curve shows the time that seperation occurs and curve becomes flat.

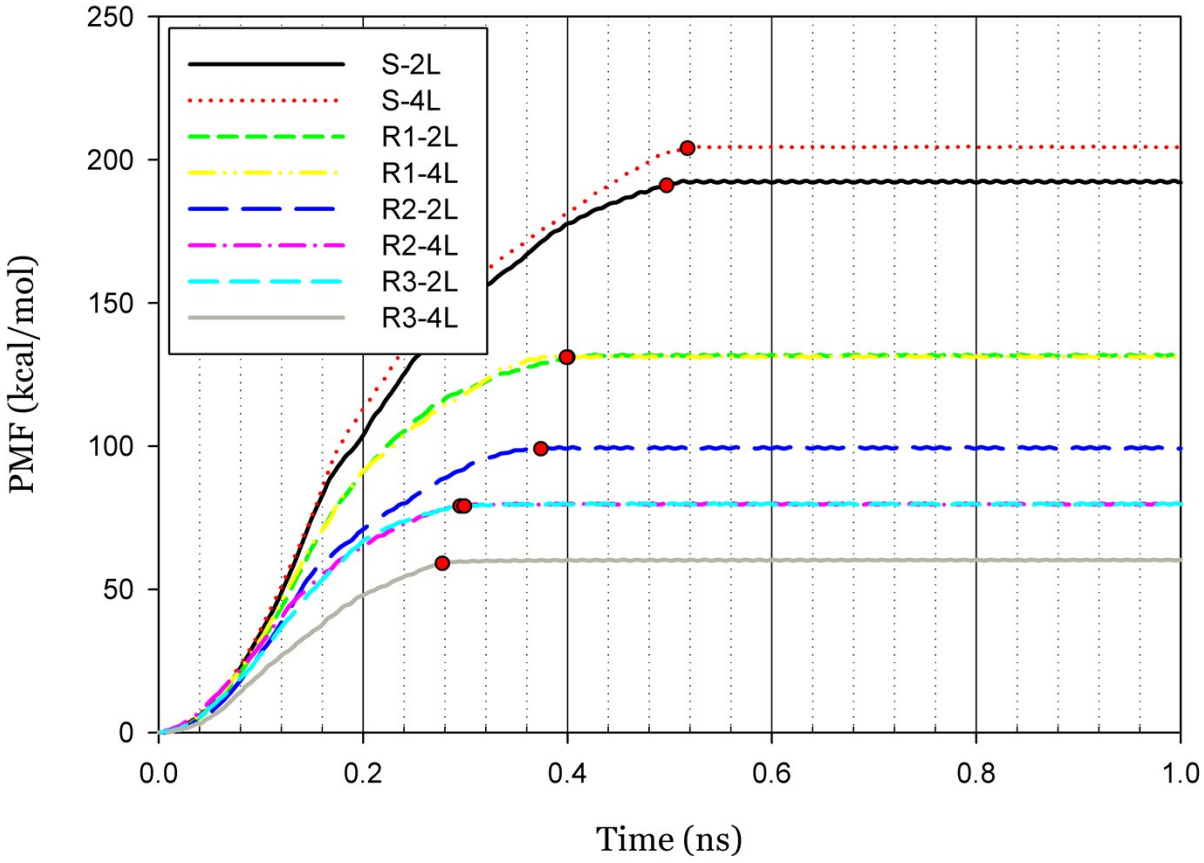

Figure S2. The PMF of water removal from the substrate versus time for different systems.

Figure S3 shows the variations of the nanodroplet contact angle during the simulation for different systems, which measured by circle fitting method.

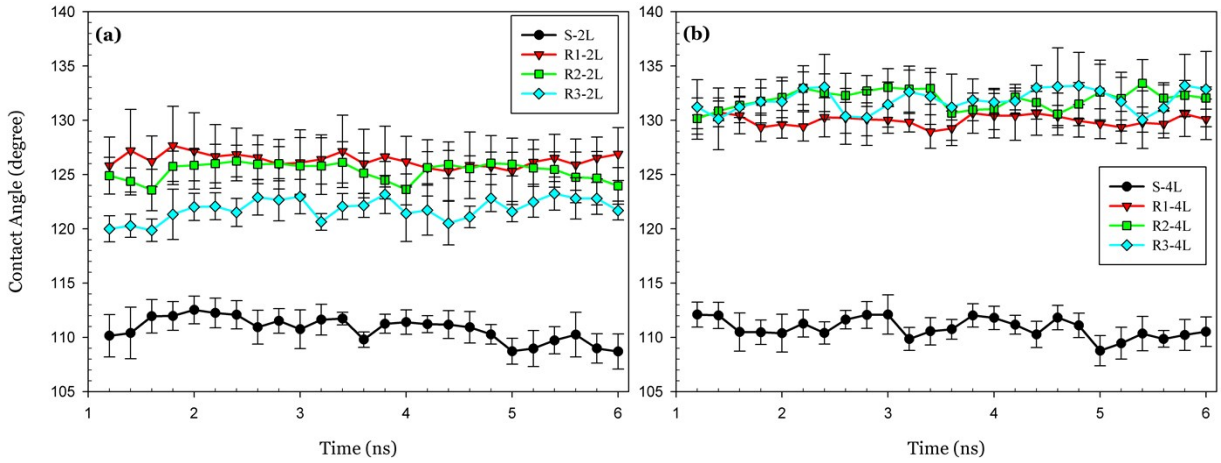

Figure S3. The nanodroplet contact angle for different systems: (a) two-layer substrates. (b) four-layer substrates.

To account the number of hydrogen bond (HB), a geometrical criterion was used, which is shown in figure S4. In this method, a HB was formed if $R_{OO} \leq 3.5$ Å (R_{OO} is the distance between oxygen atoms of donor and acceptor molecules), $R_{OH} \leq 2.4$ Å (R_{OH} is the distance between hydrogen atom of donor molecule and oxygen atom of acceptor molecule) and $\phi \leq 30^{\circ}$ (ϕ is the angle between O-H bond in donor molecule and direction of connecting line between oxygen atoms of donor and acceptor molecules). The values of R_{OO} and R_{OH} were determined by analyzing the radial distribution function of nanodroplets.

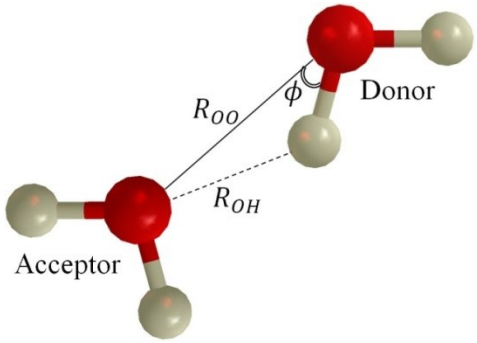

Figure S4. Schematic representation of the geometrical criterion to calculate the number of hydrogen bond.

Figure S5 shows the hydrogen bond lifetime (τ_{HB}) in the whole of the nanodroplet and in the contact layer.

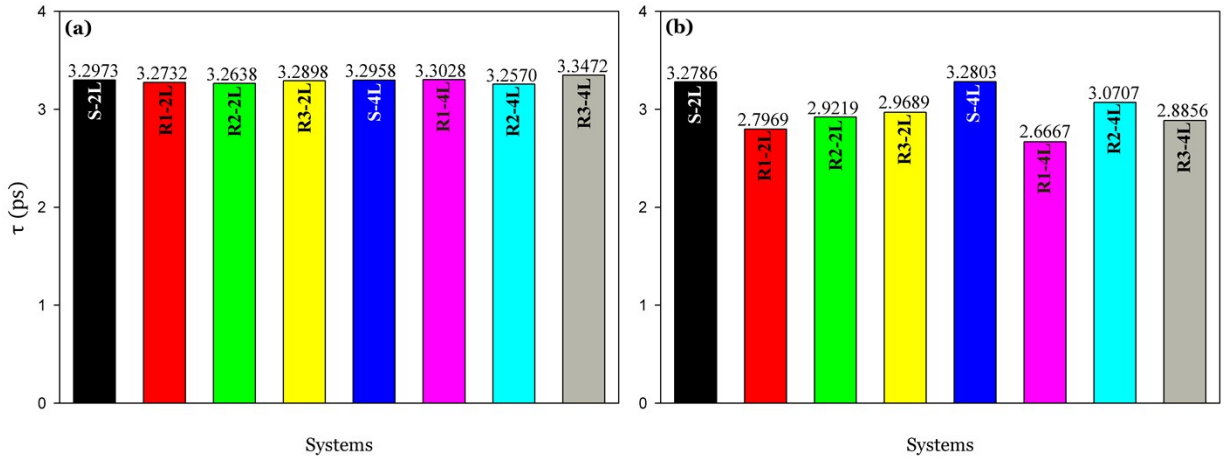

Figure S5. Hydrogen bond lifetime (a) in the whole of the nanodroplet and (b) in the contact layer.