Supplementary Information

Unidirectional Transport of Water Nanodroplet Entrapped inside Nonparallel Smooth Surface: A Molecular Dynamics Simulation Study

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**Figure S1:** Different types of NPS with different surface angle (θ) and separation distance (S).

**Table S1:** Table containing information about the surface angle (θ) and separation distance (S) of different types of NPS.

| Type of NPS | Surface Angle “θ” (°) | Separation Distance “S” (Å) |
|-------------|------------------------|----------------------------|
| A1          | 5                      | 30                         |
| A2          | 7                      | 40                         |
| A3          | 9                      | 50                         |
| A4          | 11                     | 60                         |
| A5          | 13                     | 70                         |
**Table S2:** Table containing information about the effect of surface energy on water bridge formation between two NPSs containing 3000, 4000, 5000 and 6000 molecules.

| Surface Energy (meV) | Type of NPS Bridge Formation (for 3000 water molecule droplet) |
|---------------------|---------------------------------------------------------------|
|                     | A1 | A2 | A3 | A4 | A5 |
| 7.5                 | Yes| Yes| Yes| Yes| No |
| 17.5                | Yes| Yes| Yes| Yes| No |
| 27.5                | Yes| Yes| No | No | No |
| 37.5                | Yes| Yes| No | No | No |

| Surface Energy (meV) | Type of NPS Bridge Formation (for 4000 water molecule droplet) |
|---------------------|---------------------------------------------------------------|
|                     | A1 | A2 | A3 | A4 | A5 |
| 7.5                 | Yes| Yes| Yes| Yes| Yes|
| 17.5                | Yes| Yes| Yes| Yes| No |
| 27.5                | Yes| Yes| No | No | No |
| 37.5                | Yes| Yes| No | No | No |

| Surface Energy (meV) | Type of NPS Bridge Formation (for 5000 water molecule droplet) |
|---------------------|---------------------------------------------------------------|
|                     | A1 | A2 | A3 | A4 | A5 |
| 7.5                 | Yes| Yes| Yes| Yes| Yes|
| 17.5                | Yes| Yes| Yes| Yes| No |
| 27.5                | Yes| Yes| No | No | No |
| 37.5                | Yes| Yes| No | No | No |

| Surface Energy (meV) | Type of NPS Bridge Formation (for 6000 water molecule droplet) |
|---------------------|---------------------------------------------------------------|
|                     | A1 | A2 | A3 | A4 | A5 |
| 7.5                 | Yes| Yes| Yes| Yes| Yes|
| 17.5                | Yes| Yes| Yes| Yes| No |
| 27.5                | Yes| Yes| No | No | No |
| 37.5                | Yes| Yes| No | No | No |

**Table S3:** Table containing information about the effect of surface energy on water contact angle on flat surface and its respective interaction with the solid surface.

| Surface Energy (meV) | Water Contact Angle (°) | Interaction Energy (meV/molecule) |
|----------------------|-------------------------|-----------------------------------|
| 7.5                  | 110.4                   | -3.132                            |
| 17.5                 | 83.5                    | -8.704                            |
| 27.5                 | 64.3                    | -15.477                           |
| 37.5                 | 40.2                    | -25.708                           |