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Nanoscale Capillary Bridges and the Role of Hydration Forces[1]
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This talk presents results from theoretical and numerical analysis of a nano water bridge (of height 1 to 10 nm) studied via both fully atomistic molecular dynamics (MD) simulations and continuum-based models based on the Young-Laplace equation. For nanoscale separations between two flat walls, surface forces (e.g., van der Waals and hydration forces) significantly affect the capillary bridge shape, as well as the liquid-solid contact area and contact angle. Nevertheless, the local radius of the capillary bridge is reasonably well described by the classical Young-Laplace equation for surprisingly small heights of about 3 nm (i.e., 10 molecular layers). On the other hand, the curvature predicted by the classical Young-Laplace equation is constant and differs significantly from that reported by MD simulations. As a result, when the water bridge height is smaller than 5-10 nm we observe large differences between adhesion forces obtained from MD simulations and those predicted by Young-Laplace. To accurately account for results from fully atomistic MD simulations we must extend the Young-Laplace description by including a disjoining pressure that considers hydration forces associated with molecular layering and structural changes in the water near the walls.

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