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Thermodynamics and kinetics of wetting transition of an oily fluid on surfaces with nanoscale roughness: A molecular dynamics study ELIZABETH SAVOY[1], FERNANDO ESCOBEDO, Cornell University — Surface wettability has garnered significant interest in recent years, as design and manufacture of nanoscale features allows fabrication of highly non-wetting surfaces. Such behavior is more difficult to achieve for low surface-tension fluids such as oils, and requires novel approaches. One approach is to create roughness features that provide an energy barrier to the fluid's transition from the composite to fully wetted state. We use molecular dynamics of small droplets in combination with various simulation techniques, such as umbrella sampling and forward flux sampling, to probe the energy landscape associated with the wetting transition and compute transition rates and their dependence on key topological parameters such as feature height. We find that the drop does not transition with a flat liquid-vapor interface when it penetrates and wets the subsurface features (as is often assumed in continuum treatments) and that the hysteresis in the wetting and dewetting transitions is associated with differences in the evolution of that interface.

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