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Comparing atomistic hydrate and ice adhesion on solid surfaces

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Despite seemingly similar to ice, gas hydrate exhibits much weaker adhesion to solid surfaces. Understanding the atomistic adhesion of hydrate on solid surfaces, and further comparing it to ice adhesion, can shed light on the fundamentals of novel anti-hydrate materials design. In this work, large-scale molecular simulations are employed to investigate the adhesion of hydrate particles on solid surfaces, especially with focuses on the atomistic structures and the corresponding influences of an interfacial adhesion layer. The results indicate that strong hydrogen bonding can induce the growth of hydrate lattice in interfacial liquid water molecules unless the substrate can trigger ice nucleation and replace the empty cage in the process of competitive growth. By comparing tensile detaching ice and hydrate from solid surfaces, it is found that the variation in the lattice form of water molecules and the adsorption layer of guest molecules are the microscopic reasons for the lower adhesion strength of hydrate.