# Interpretation of Young's equation from a nanoscale viewpoint: mechanical and thermodynamic routes toward the understanding of wetting

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Wetting has long been a topic of interest in various science and engineering fields because it plays a key role in the wetting properties. It includes the behavior of the so-called contact line (CL), where a liquid-vapor (or liquid-gas) interface meets a solid surface., and by introducing the concept of interfacial tensions, Young's equation first proposed in 1805 is commonly used with the contact angle as a measure of wettability at the macroscopic scale.

We carried out molecular dynamics (MD) simulations of an equilibrium contact line (CL) of a Lennard-Jones fluid on a flat and smooth solid surface [1], on a flat surface of a boundary of wettability [2], as well as of a nonequilibrium CL moving on a flat surface [3], where we extracted the fluid stress-tensor distribution, and examined the force balance in the surface-lateral direction exerted on a rectangular control volume set around the contact line. As the mechanical route shown in Fig. 1, the fluid stress integrals along the two control surfaces normal to the solid-fluid interface were theoretically connected with $\gamma_{SL}$ and $\gamma_{SV}$ relative to the solid-vacuum interfacial tension $\gamma_{S0}$ by Bakker's equation extended to solid-related interfaces via a thought experiment. On the other hand, the fluid stress integral along the control surface lateral to the solid-fluid interface was connected with $\gamma_{LV}$ by the Young-Laplace equation. Through this connection, we showed that Young's equation was valid for a system in which the net lateral force exerted on the fluid molecules from the solid surface was zero around the contact line. Furthermore, we compared the interfacial tensions obtained by the mechanical route with the solid-liquid and solid-vapor works of adhesion obtained by the dry-surface method as one of the thermodynamic routes, and showed that both routes resulted in a good agreement. These results also indicated that the contact angle should be predicted not only by the interfacial tensions but also by the pinning force exerted around the contact line [2] (Fig. 2). This connection of the mechanical and thermodynamic routes were extended to the analysis of a dynamic CL [3] as well as a more realistic fluid-solid pair, e.g., water on $SiO_2$ surface [4].

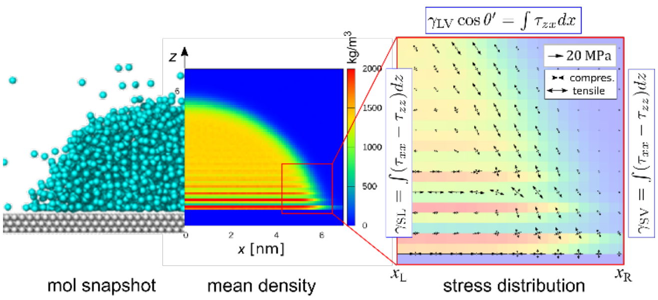


**Figure 1:** Connection of microscopic stress distribution with macroscopic interfacial tensions.

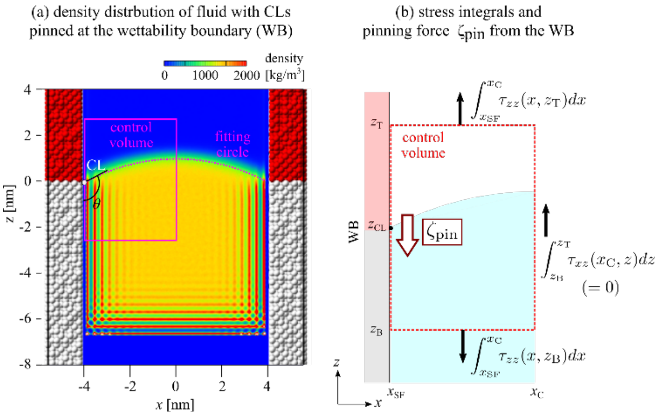


**Figure 2:** Understanding of Young's equation under the existence of pinning force exerted on the fluid around the contact line. Reprinted with permission from Kusudo *et al.*, J. Chem. Phys. **151**, 154501 (2019). Copyright 2019 Author(s), licensed under a Creative Commons Attribution (CC BY) license 4.0 License.

## References

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**4.** D. Surblys *et. al.*, J. Chem. Phys. **148**, 134707 (2018).