Surface Free Energy Characterization of Soft Materials through Computational Experiments

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ABSTRACT

The surface free energy of soft coatings determines the adhesion, friction, and wettability response of solid surfaces in several applications of engineering and biomedical interest. However, the multiscale nature of these phenomena limits a bottom-up prediction of the resulting surface properties.

In this work we use computational experiments to characterize the surface and solid-fluid interface of low-surface-free-energy coatings and materials. In particular, the free energy perturbation approach is first used to evaluate the work of adhesion between polymer surfaces and fluids; then, the Young-Dupré equation is adopted to compute the ideal contact angle. Such molecular dynamics and coarse-grained simulations allow to explore the interfacial properties of soft materials, enabling a more comprehensive understanding of their effect on the adhesion, friction, and wettability of solid surfaces. Differently from standardized experimental approaches, numerical experiments allow to understand and decouple the different mechanisms regulating the wetting properties of soft coatings with atomistic precision. The aim is to propose a first step towards a multiscale standard framework for the computational characterization of surfaces, required for the optimal design of super-hydrophobic materials.

The results obtained in this work will be used as input parameters for materials modeling at higher scales, such as finite elements simulations, to investigate the contribution of surface topology on wettability, in terms of nano- and micro-roughness or patterning. In perspective, multiscale models linking the chemical and topological characteristics of soft surfaces with their effective response will allow predictive in silico testing of new materials with tunable functionalities.

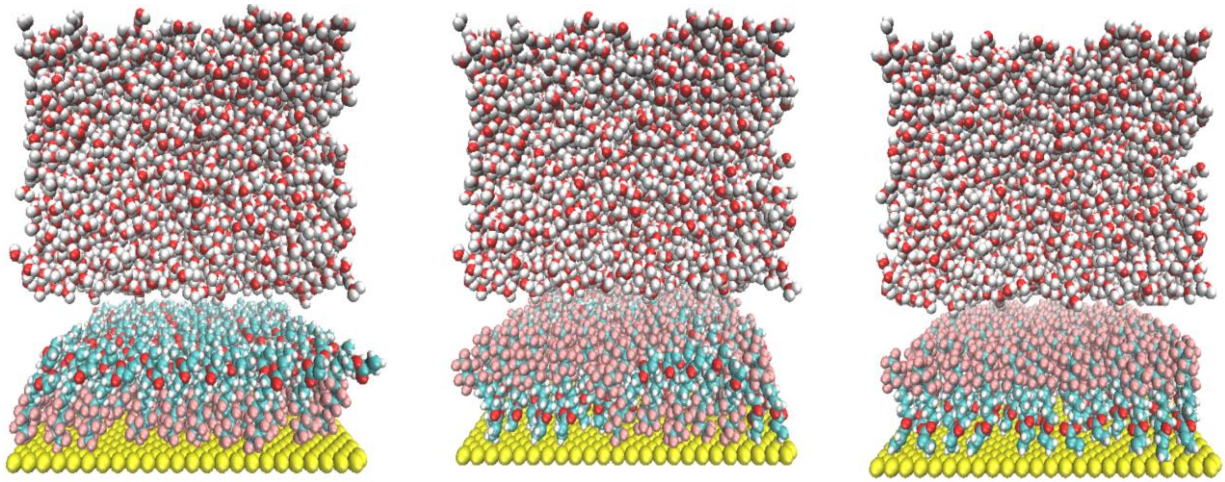

Figure 1. Different coatings of a solid surface in contact with water modelled by atomistic simulations.