Soft Materials Surface and Interface Characterization Through Molecular Dynamics Simulations

Francesco Maria Bellussi [S], Annalisa Cardellini, Pietro Asinari and Matteo Fasano [C]
Department of Energy, Politecnico di Torino, Torino, Italy
matteo.fasano@polito.it

In this work we use Molecular Dynamics (MD) simulations to characterize the surface and the interface of low free energy materials. In particular, we use first the Free Energy Perturbation (FEP) approach to evaluate the work of adhesion between polymer surfaces and different solvents, and then the Young-Dupré equation to compute the ideal contact angle. Furthermore, the MD simulations carried out in this work allow to explore the interfacial properties between two soft materials, enabling a more comprehensive understanding of wettability phenomena on soft surfaces. On one hand, our results clarify the surface and interface behaviors of polymers, and on the other hand provide some insights on the chemical and physical contribution on the wetting properties, differently from the standardized experimental approaches. Then, the aim is to propose the first step towards a multiscale standard framework for the surface characterization, required for the optimal design of super-hydrophobic materials. The results obtained in this work will be used as input parameters for the modeling activities at higher scales, such as coarse graining and finite elements simulations, to investigate the physical contributions to the wettability properties, in terms of nano and micro roughness or patterning. Our results are finally compared with experimental data obtained from samples chemically equivalents to the models proposed at the atomistic level. This work is funded by the H2020 project OYSTER (grant number 760827).