**Nanostructured surfaces**

**Three wetting modes of nanostructured surfaces by liquid in coarse-grain approach**

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Understanding of a solid surface wetting by a liquid has important practical appliance and technological relevance in various applied areas. Particularly, it is significantly relevant for achieving efficient surface modification. Thus, physical and chemical insight regarding interfacial phenomena at the nanoscale is certainly essential.

Molecular dynamics is a versatile tool for investigation of effects occurring at the interface between different phases. The main advantages of this methods arise because of the possibilities of interface reconstructing at the atomistic level. Nevertheless, important computational resources required for simulations are strong drawbacks of its more intensive application at the microscale. Therefore, the use of coarse-grained molecular dynamics approaches start to be more and more demanded. However, the selection of a specific coarse-grained model is dependent on the concrete physics of the system under investigation. Thus, some additional study of interactions between atoms of different species and phases is significant to represent well properties of the system.

In our report, we considered a nanoscale water droplet located on the structured solid surface. For representation of a water molecule, we use one-site coarse-grained electrically-based ELBA model [1]. The wetting states of the droplet depending on the features of surface structuration were under investigation. Thus, a two cases of structuration (nanoporous silicon surface and silicon surface with nanopillars) were chosen. We studied the three modes of wetting regimes: the first one is the hydrophilic $(θ=60^{o})$ , the second one is neutral $(θ=88^{o}$), and the third case corresponds to a hydrophobic wetting mode ($θ=120^{o}$). With the variation of the parameters of interactional potential, we considered applicability of Wenzel's and Cassie–Baxter models for wetting angle [3]. We revealed that the structuration influence on variation of wetting properties in different ways depending on the initial wetting regime. Particularly, the structuration under hydrophilic (hydrophobic) mode of wetting leads to increase of hydrophilicity (hydrophobicity). For neutral wetting mode, the regimes of hydrophilicity and hydrophobicity can be realized. We adopted an analytical model proposed previously by Kim, Pugno and Ryu [2] for the study of impact of the specific surface rise due to the structuration. This model can explain an improvement of hydrophilicity (hydrophobicity), nevertheless even if the model gives the same range of value of contact angle, the behavior of the dependency of wetting angle on roughness is not represented well. The difference can be explained by the pining of contact line and resulting hysteresis of contact angle.

[1] M. Orsi and J. W. Essex, “The ELBA force field for coarse-grain modeling of lipid membranes,” *PLoS One*, vol. 6, no. 12, 2011.

[2] D. Kim, N. M. Pugno, and S. Ryu, “Wetting theory for small droplets on textured solid surfaces,” *Sci. Rep.*, vol. 6, no. May, pp. 1–8, 2016.

[3] A. Marmur, “Wetting on hydrophobic rough surfaces: To be heterogeneous or not to be?,” *Langmuir*, vol. 19, no. 20, pp. 8343–8348, 2003.