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Modeling Wettability and Friction of Water on MoS_2 Surface BINQUAN LUAN, RUHONG ZHOU, IBM T J Watson Res Ctr — The molybdenum disulfide (MoS_2) nanosheet is a promising new two-dimensional (2D) material and has recently been used in biological sensing. While the electronic strudture of 2D MoS_2 sheet has been extensively studied, the role of its atomic structure and thus the interfacial interactions with bio-fluids are still elusive. Using Molecular dynamics simulations, we modeled the contact angle of water on the MoS_2 nanosheet and predicted the slip-length of water (that is not measurable in experiment yet). Simulation results suggest that the MoS_2 nanosheet is a hydrophobic and low-friction surface. We expect that our newly developed force fields for depicting surface atoms of MoS_2 will facilitate future research in understanding biomolecule-MoS_2 interactions in MoS_2-based biosensors.

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