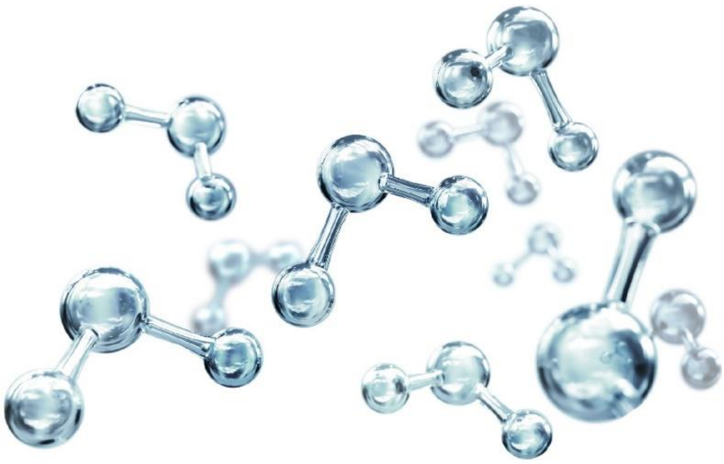
Seminar

6th of December 2024
11:00 h

In person meeting at DESY!
CFEL, Building 99, room SR4



Zoom Virtual Meeting:
https://tuhh.zoom.us/j/82631283465
Meeting-ID: 826 3128 3465
Password: 978444

Prof. Dr. Roland R. Netz
Freie Universität Berlin

Water, acids and bases at interfaces: graphene versus air

The interfacial properties of water and water ions are important for many technological and biological applications. Studies of air-water and graphene-water interfaces have been instrumental for advancing our understanding of aqueous interfaces, but many open questions remain. Experimental water contact angles show extreme variations among reported values for graphene and a clustering into groups for freshly exfoliated (60° ± 13°) and not-freshly exfoliated graphite surfaces, presumably due to contamination effects. Based on this 60° graphite-water contact angle we derive a contact angle for unsupported graphene of 80°, in agreement with the experimental observation of water entering graphene nanostructures [1]. From ab initio simulations the propensity of water ions to graphene is derived. Similarly to the interface with air, hydronium is attracted to graphene while hydroxide is repelled, caused by interface-specific hydrogen bonding: thus, the graphene surface free energy is predicted to decrease for acids and to increase for bases [2]. While graphene substantially changes the water structure and dynamics, as shown by predicted linear and non-linear water spectra at graphene, interfacial energies and electrostatic interfacial potentials are rather similar to the interface with air. Thus, graphene is slightly hydrophilic yet exhibits interfacial properties rather similar to the air interface. The thickness over which the water structure and dynamics at an interface differs from bulk water was recently determined by spatially resolved non-linear spectroscopy and found to be substantially below a nanometer, in agreement with theoretical predictions [3].

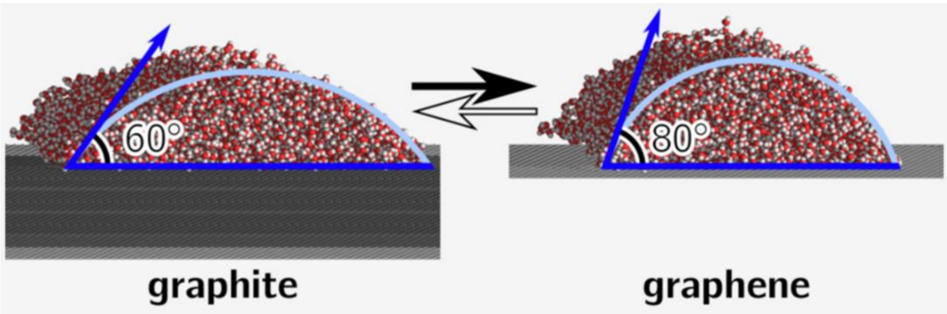


Figure 1: The water contact angle at graphene increases slightly compared to graphite yet stays below 90°, indicative of a slightly hydrophilic surface.

References:

[1] Modeling Water Interactions with Graphene and Graphite via Force Fields Consistent with Experimental Contact Angles, Shane R. Carlson, Otto Schullian, Maximilian R. Becker, and Roland R. Netz, J. Phys. Chem. Lett. 2024, 15, 6325−6333.
[2] Multiscale Modeling of Aqueous Electric Double Layers, Maximilian Becker, Philip Loche, Majid Rezaei, Amanuel Wolde-Kidan, Yuki Uematsu, Roland R. Netz, and Douwe Jan Bonthuis, Chem. Rev. 2024, 124, 1−26.
[3] How Thick is the Air−Water Interface? A Direct Experimental Measurement of the Decay Length of the Interfacial Structural Anisotropy. Alexander P. Fellows, Álvaro Díaz Duque, Vasileios Balos, Louis Lehmann, Roland R. Netz, Martin Wolf, and Martin Thämer, Langmuir 2024, 40, 18760−18772.