Molecular simulations of the wettability of Graphene and Graphite

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Abstract (Century Gothic 11)

The water wettability of carbon surfaces, such as graphene and graphite, has been extensively discussed over the past few years due to its broad range of applications. [1] Experimentally however it is difficult to untangle the effect that impurities, surface defects and number of layers have on the wetting properties. Here using molecular dynamics we report the wetting behavior of graphitic surfaces–water interfaces through the calculation of the local stress tensor based on the Irving–Kirkwood–Noll theory. We compare the interfacial properties of fully wetted and partially wetted graphene and graphite and observe that the wettability is the result of a fine balance between van der Waals (vdW), electrostatic interactions and hydrogen bonds structure.[2] We then explore how 2D confinement changes graphite wettability and the possible consequences that such changes have on water flux properties. [3]

References

[1]   D. Parobek and H. Liu, 2D Materials, 2 (2015), 032001
[2]   JD Elliott et al., J. Mater. Chem. C, 10 (2022) 15225
[3]   M. Chiricotto et al., J. Chem. Phys. C, 125, 10 (2021) 6367
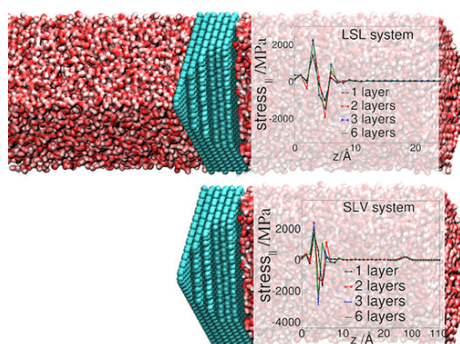[4]   Z. Wei, Carbon, 198 (2022) 132

Figure

Figure 1: Fully wetted and partially wetted graphite slabs. Corresponding surface tension plots as a function of the number of graphene layers.