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Structure and dynamics of water nano-droplets on graphene MING MA, ANGELOS MICHAELIDES, GABRIEL AEP-PLI, London Centre for Nanotechnology, University College London — The wettability of graphene and the diffusion of water droplets across it is of central importance to many emerging applications in nanofluidics. Here we report an extensive set of molecular dynamics simulations for water clusters of varying sizes on graphene (20 to 2,000 water molecules), using force field parameters fitted to recent ab initio quantum Monte Carlo data [J. Ma, A. Michaelides, D. Alfe, L. Schimka, G. Kresse, and E. G. Wang, *Phys. Rev. B* 84, 033402 (2011)]. The contact angle for the water droplets obtained here, with our ab initio water - carbon interaction, is in very good agreement with experiments. A strong size dependence in the diffusion of the water droplets across the surface is also observed. This work is a step towards understanding surface transportation in carbon based nanofluidics.

Prefer Oral Session
 Prefer Poster Session

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