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Simulation And Modeling Of Wetting And Adsorption Phenomena Associated With Nanomaterials

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Summary

Atomic Force Microscopy of hydrophobic material surfaces in water shows the presence of closely spaced soft domains. The radii of curvature of these features are of the order of 100 nm and their heights above the substrate are in the range 20-30 nm. The consensus interpretation of these features is that they are nanosized gas bubbles formed on the substrate following immersion. Levy et al.1 have shown experimentally that when graphene is stretched to form nanobubbles on a platinum substrate, electrons behave as if they are subject to magnetic fields in excess of 300 Tesla, even though no magnetic field has actually been applied. The ability to make electrons behave as if they were in magnetic fields of 300 Tesla or more - merely by stretching graphene - offers a new approach for important applications relating to modern solid state devices. There still remains the difficulty of explaining the apparent stability of nanobubbles with conventional thermodynamics.2-3 Zhou et al.,4 in their study on interfacial wetting at epitaxial graphene, have extended some of our results. An interesting result from this work, with its combined use of experimental and computational approaches, was that the macroscopic contact angle of water on epitaxial graphene layers is correlated with the number of layers. Based on their results, the small amount of the epitaxial buffer layer of bi-layer graphene that makes direct contact with water helps explain its macroscopic contact angle being close to the value for bulk graphite, that is
{}{} . This contact angle value for bulk graphite, independent of the number of graphene layers, n, was also obtained after it was found that the water-exposure coverage of Gn (n-layer graphene) was close to unity. These results agree with ours,5specifically the room temperature contact angle value of water on graphite. On another front, we note that recent experiments have found evidence for phase transitions of gases (e.g. argon and krypton) adsorbed on a single carbon nanotube. In order to understand these observations, classical Grand Canonical Monte Carlo simulations have been performed.3 Intricate and overlapping nanoscale issues relating to the modeling and simulation of wetting phenomena, formation of nanobubbles on nanomaterials, and the adsorption of rare gas atoms in carbon nanotubes, will be compared and discussed.

1 N. Levy et al., Science 329, 544-547 (2010).

2 Fundamentals and Current Topics in Molecular Structure Research, P. Misra and

C. Haridas (Editors), Research Signpost, 2011.

3M. Mercedes et al., in Adsorption by Carbons, E.J. Bottani and J.M.D. Tascon (Editors), Elsevier Science Publishing, pp. 187-210, 2008.

4Hua Zhou et al., "Understanding controls on interfacial wetting at epitaxial graphene: Experiment and theory", Physical Review B, (85), pp. 035406-1 - 035406-11, 2012.

5H. Elnaiem, D. Casimir, P. Misra, S. M. Gatica., "Nanobubbles at Water-Solid Interfaces: Calculation of the Contact Angle Based on a Simple Model", Computers Materials & Continua (CMC) (368), no. 1, pp. 1-12, Tech Science Press, (2009).