Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Nanodroplets of immiscible fluid pairs adopt nonspherical shapes[1]
GERALD WILEMSKI, Missouri University of Science and Technology, FAWAZ HRAHSHEH, King Fahd University of Petroleum and Minerals and Missouri University of Science and Technology — To help understand recent experimental results for nonane/water condensation [Pathak, et al. J. Chem. Phys. **140**, 224318 (2014)], the structure of water/nonane nanodroplets was investigated using classical molecular dynamics (MD) simulations of SPC/E water and a unified atom model of nonane. Because nonane and water are essentially immiscible fluids that only partially wet each other, one might expect unusual nanodroplet structures to arise. Indeed, nonspherical, phase-separated Russian Doll (RD) structures were found to occur for these nanodroplets over the entire temperature range studied in the MD simulations, 220K – 300K. An idealized, but realistic lens-on-sphere model for the observed RD structures consists of a spherical nonane lens that partially wets a spherical water droplet. This model was used to analyze the experimental small angle x-ray scattering measurements. The simulated contact angle of nonane on water was found to be quite sensitive to the value of the Lennard-Jones energy parameter ε_{OC} for the cross-interaction between oxygen and carbon atoms. The standard geometric mean approximation for ε_{OC} yielded contact angles in the range 70^o- 80^o, while a 19% increase in ε_{OC} reduced the simulated contact angle close to the experimental value of 33.6^o at 295 K.

[1]Supported by NSF Grant No. CBET-1033387

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Date submitted: 14 Nov 2014 Electronic form version 1.4