Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Wetting transitions in alkane-water systems for nanodroplets and planar interfaces PAUF NEUPANE, Missouri University of Science and Technology, FAWAZ HRAHSHEH, King Fahd University of Petroleum and Minerals and Missouri University of Science and Technology, GERALD WILEMSKI, Missouri University of Science and Technology — The temperature dependent wetting behavior of alkanes on water is studied using molecular dynamics simulations for SPC/E water and unified atom 6-12 Lennard-Jones (LJ) alkane models. Water-alkane interactions are modeled using a LJ potential with energy and size parameters adjusted to reproduce experimentally observed wetting behavior for nonane at 295 K. For reasonable values of the LJ parameters, core-shell structures of water-nonane nanodroplets are observed at low temperatures, T <250 K, indicating that nonane perfectly wets SPC/E water with a zero contact angle at low temperatures. At higher T, imperfect wetting is found as a nonane lens forms on the water drop with a finite, non-zero contact angle yielding a Russian Doll structure. For planar alkane-water interfaces, our simulation results are consistent with the occurrence of low temperature and high temperature wetting transitions. Within the imperfect wetting region at low temperature, the contact angle formed by alkanes on water initially increases with temperature until a maximum dewetting temperature (MDT) is reached. Beyond the MDT, the contact angle decreases as the system approaches the usual high temperature wetting transition. The imperfect wetting temperature range decreases with reducing alkane chain length.

Pauf Neupane
Missouri University of Science and Technology

Date submitted: 13 Nov 2016 Electronic form version 1.4