Abstract Submitted
for the DFD16 Meeting of
The American Physical Society

Nanodrop contact angles from molecular dynamics simulations SRIKANTH RAVIPATI, BENJAMIN AYMARD, PETR YATSYSHIN, Complex Multiscale Systems Group, Department of Chemical Engineering, Imperial College London, AMPARO GALINDO, Centre for Process Systems Engineering Group, Department of Chemical Engineering, Imperial College London, SERAFIM KALLIADASIS, Complex Multiscale Systems Group, Department of Chemical Engineering, Imperial College London — The contact angle between three phases being in thermodynamic equilibrium is highly sensitive to the nature of the intermolecular forces as well as to various fluctuation effects. Determining the Young contact angle of a sessile drop sitting on a substrate from molecular dynamics (MD) simulations is a highly non-trivial task. Most commonly employed methods for finding droplet contact angles from MD simulation data either require large numbers of particles or are system-dependent. We propose a systematic geometry based methodology for extracting the contact angle from simulated sessile droplets by analysing an appropriately coarse-grained density field. To demonstrate the method, we consider Lennard-Jones (LJ) and SPC/E water nanodroplets of different sizes sitting on planar LJ walls. Our results are in good agreement with Young contact angle values computed employing test-area perturbation method.

Srikanth Ravipati
Complex Multiscale Systems Group, Department of Chemical Engineering, Imperial College London

Date submitted: 30 Jul 2016 Electronic form version 1.4