submitted to *Phys. Chem. Chem. Phys.* on April 9, 2007

Dumbbells and Onions in Ternary Nucleation

Ricky B. Nellas,[a] Bin Chen,[a,*] and J. Ilja Siepmann[b,*]

[a]Department of Chemistry, Louisiana State University
Baton Rouge, Louisiana 70803-1804, U.S.A.

[b]Departments of Chemistry and of Chemical Engineering and Material Science
and Supercomputing Institute, University of Minnesota,
207 Pleasant Street SE, Minneapolis, Minnesota, 55455-0431, U.S.A.

Abstract

Molecular simulations for a ternary nucleation system (water/n-nonane/1-butanol) demonstrate a more complex nucleation mechanism than previously thought, where critical nuclei with different compositions are present even for a given vapour-phase composition; the spatial distribution in these critical nuclei is heterogeneous and dumbbell and onion motifs are found; in the former, water and nonane nano-droplets are connected through a butanol handle, while in the latter a water core is surrounded by a nonane corona with an interfacial butanol shell.