Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Molecular Dynamics simulation of Oil-Water liquid-liquid interfaces JANAMEJAYA CHOWDHARY, Department of Chemistry, Colorado State University, BRANKA LADANYI, Department of Chemistry, Colorado State University — Molecular Dynamics simulations are performed water-hydrocarbon liquid systems to study the effect of hydrocarbon branching on interfacial properties.The following two series of hydrocarbons are considered: 1) n-octane, 2-methyl heptane and 2,2,4 trimethyl pentane (constant molecular mass), and 2) n-pentane, 2-methyl pentane and 2,2,4 trimethyl pentane (constant chain length). The density profiles were constructed and analyzed in terms of the Capillary Wave model. With a simple algorithm for identification of surface molecules at the interface, intrinsic density profiles were obtained for different systems and found to resemble density profiles of a liquid in the presence of a soft wall. This supports the picture of a sharp interface broadened by capillary waves. Order parameters are used to study the orientation of water and hydrocarbon molecules corresponding to the total and intrinsic density profiles. At the interface, water preferably points one O-H bond towards the hydrocarbon, linear hydrocarbons stack parallel to, while the more branched hydrocarbons orient perpendicular to the interface.

Janamejaya Chowdhary
Colorado State University

Date submitted: 01 Dec 2004 Electronic form version 1.4