Liquid-Liquid Interface in Simulation

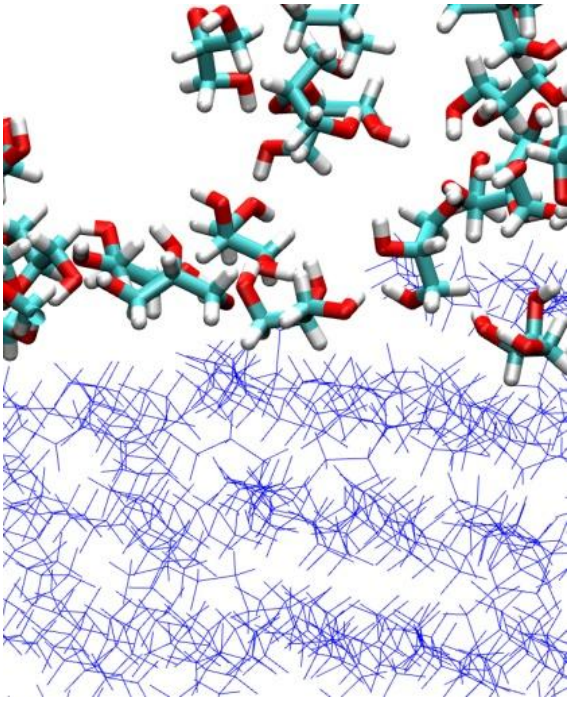
Andreas Krause,[a,b,‡] Frank R. Beierlein,[a,b,‡] Christof M. Jäger,[a,b] Piotr Fita,[c,d] Eric Vauthey[c] and Timothy Clark*[,a,b]

[a] Computer-Chemie-Centrum and Interdisciplinary Center for Molecular Materials, Friedrich-Alexander-Universität Erlangen-Nürnberg, Nägelsbachstr. 25, 91052 Erlangen, Germany

[b] Excellence Cluster Engineering of Advanced Materials, Friedrich-Alexander-Universität Erlangen-Nürnberg, Nägelsbachstr. 49b, 91052 Erlangen, Germany

[c] Department of Physical Chemistry, University of Geneva, 30 quai Ernest-Ansermet, CH-1211 Geneva 4, Switzerland

[d] Institute of Experimental Physics, Faculty of Physics, University of Warsaw, ul. Hoza 69, 00-681 Warsaw, Poland



Interfaces, at which different phases are in close contact, are of special interest because the properties of the molecules at the interface can differ decidedly from those in the bulk. Due to the asymmetry of the forces, molecules at interfaces are frequently observed to be more ordered than in the bulk, where more random orientations are usually observed. [1,2] As a result, even such fundamental characteristics as pH and equilibrium constants can differ dramatically.

While it is difficult to probe interfaces with linear optical spectroscopy because of the preponderance of molecules in the bulk, non-linear optical techniques such as Second Harmonic Generation (SHG), have been used increasingly to study interfaces in recent years.[3,4]

Experimental SHG-measurements were performed on a glycerol/water dodecane interface.[5,6] In order to obtain a detailed view of the interface structure, we have performed extensive molecular-dynamics simulations of a two-phase system formed by glycerol/water and dodecane, with MG and BG at the interfaces, and over a wide range of glycerol concentrations.

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