Abstract Submitted
for the DFD17 Meeting of
The American Physical Society

Transport properties at fluids interfaces: a molecular study for a macroscopic modelling ANTONIO RUSSO, Imperial College London, MATTEO MORCIANO, Politecnico di Torino, DAVID N. SIBLEY, Loughborough University, ANDREAS NOLD, Max Planck Institute for Brain Research, BENJAMIN D. GODDARD, The University of Edinburgh, PIETRO ASINARI, Politecnico di Torino, SERAFIM KALLIADASIS, Imperial College London — Rapid developments in the field of micro- and nano-fluidics require detailed analysis of the properties of matter at the molecular level. But despite numerous works in the literature, appropriate macroscopic relations able to integrate a microscopic description of fluid and soft matter properties at liquid-vapour and multi-fluid interfaces are missing. As a consequence, studies on interfacial phenomena and micro-device designs often rely on oversimplified assumptions, e.g. that the viscosities can be considered constant across interfaces. In our work, we present non-equilibrium MD simulations to scrutinise efficiently and systematically, through the tools of statistical mechanics, the anisotropic properties of fluids, namely density variations, stress tensor, and shear viscosity, at the fluid interfaces between liquid and vapour and between two partially miscible fluids. Our analysis has led to the formulation of a general relation between shear viscosity and density variations validated for a wide spectrum of interfacial fluid problems. In addition, it provides a rational description of other interfacial quantities of interest, including surface tension and its origins, and more generally, it offers valuable insight of molecular transport phenomena at interfaces.

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Date submitted: 28 Jul 2017 Electronic form version 1.4