Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Nonequilibrium thermodynamics of an interface THIERRY SAVIN, University of Cambridge, MARCO SCHWEIZER, HANS CHRISTIAN ÖTTINGER, ETH Zurich — Interfacial thermodynamics has deep ramifications in understanding the boundary conditions of transport theories. We present a formulation of local equilibrium for interfaces that extends the thermodynamics of the "dividing surface," as introduced by Gibbs, to nonequilibrium settings such as evaporation or condensation. By identifying the precise position of the dividing surface in the interfacial region with a gauge degree of freedom, we exploit gauge-invariance requirements to consistently define the intensive variables for the interface. The model is verified under stringent conditions by employing high-precision nonequilibrium molecular dynamics simulations of a coexisting vapor-liquid Lennard-Jones fluid. We conclude that the interfacial temperature is determined using the surface tension as a "thermometer," and can be significantly different from the temperatures of the adjacent phases.

Thierry Savin
University of Cambridge

Date submitted: 06 Nov 2015 Electronic form version 1.4