

Abstract Submitted
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Dynamic surface tension effects from molecular dynamics simulations ALEX LUKYANOV, University of Reading — Effects of dynamic surface tension have been studied in a model system using molecular dynamics simulations. The model system has been made of an artificially expanding liquid droplet, with the rate of change of the external surface area being comparable with the gas-liquid interface formation characteristic time, obtained from the estimates of macroscopic theories. The size of the liquid droplet has been chosen to have about 5,000-7,000 identical molecules, each having between 10-20 beads, to obtain well developed and separated the bulk and surface phases. The methodology of surface tension evaluation has been verified against the Laplace Law in a stationary state of the liquid drop. The results of the MD simulations will be discussed in comparison with the estimations obtained from macroscopic experiments on dynamic wetting using a sharp interface formation theory for different chain length of molecules and strength of intermolecular interactions.

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