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Surface tension relaxation time in liquid-gas and liquid-solid interfaces of simple LJ liquids[1] ALEX LUKYANOV, ALEXEI LIKHTMAN, University of Reading — We use molecular dynamics (MD) to answer a classical question: how does the surface tension on an interface appear? After defining surface tension from the first principles and conducting several consistency checks, we perform a series of dynamic MD experiments. First, we use a single simple liquid nanodroplet to study liquid-gas (LG) interface dynamics. At time zero, we remove the outer layer of molecules in the droplet, creating a fresh bare interface with the bulk arrangement of molecules. After that the system evolves towards equilibrium, and the expected surface tension is re-established. We found that in the case of LG interfaces, the system relaxation consists of three distinct stages. We have observed this scenario for monatomic Lennard-Jones (LJ) liquids as well as for binary LJ mixtures at different temperatures, monitoring a wide range of physical observables. Second, we use an equilibrated liquid film on a solid substrate. At time zero, we change the strength of the interaction potential between the substrate and liquid molecules and observe how the liquid-solid interface evolves towards equilibrium. We apply results to representative nanoflows over chemically structured substrates and discuss implications to macroscopic modelling of dynamic contact angle.

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