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Multi-scale strategies for dealing with moving contact lines¹ EDWARD R. SMITH, Imperial College London, PANAGIOTIS THEODORAKIS, Polish Academy of Sciences, RICHARD V. CRASTER, OMAR K. MATAR, Imperial College London — Molecular dynamics (MD) has great potential to elucidate the dynamics of the moving contact line. As a more fundamental model, it can provide *a priori* results for fluid-liquid interfaces, surface tension, viscosity, phase change, and near wall stick-slip behaviour which typically show very good agreement to experimental results. However, modelling contact line motion combines all this complexity in a single problem. In this talk, MD simulations of the contact line are compared to the experimental results obtained from studying the dynamics of a sheared liquid bridge. The static contact angles are correctly matched to the experimental data for a range of different electro-wetting results. The moving contact line results are then compared for each of these electro-wetting values. Despite qualitative agreement, there are notable differences between the simulation and experiments. Many MD simulation have studied contact lines, and the sheared liquid bridge, so it is of interest to review the limitations of this setup in light of this discrepancy. A number of factors are discussed, including the inter-molecular interaction model, molecular-scale surface roughness, model of electro-wetting and, perhaps most importantly, the limited system sizes possible using MD simulation.

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Omar Matar
Imperial College London

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