

Abstract Submitted
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Dynamics of two-phase interfaces and surface tensions: A density-functional theory perspective¹ PETR YATSYSHIN, Department of Chemical Engineering, Imperial College London, London, UK, DAVID N. SIBLEY, Department of Mathematical Sciences, Loughborough University, Loughborough, UK; Department of Chemical Engineering, Imperial College London, London, UK, MIGUEL A. DURAN-OLIVENCIA, SERAFIM KALLIADASIS, Department of Chemical Engineering, Imperial College London, London, UK — Classical density functional theory (DFT) is a statistical mechanical framework for the description of fluids at the nanoscale, where the inhomogeneity of the fluid structure needs to be carefully accounted for. By expressing the grand free-energy of the fluid as a functional of the one-body density, DFT offers a theoretically consistent and computationally accessible way to obtain two-phase interfaces and respective interfacial tensions in a ternary solid-liquid-gas system. The dynamic version of DFT (DDFT) can be rigorously derived from the Smoluchowsky picture of the dynamics of colloidal particles in a solvent. It is generally agreed that DDFT can capture the diffusion-driven evolution of many soft-matter systems. In this context, we use DDFT to investigate the dynamic behaviour of two-phase interfaces in both equilibrium and dynamic wetting and discuss the possibility of defining a time-dependent surface tension, which still remains in debate.

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