Hydrophobicity: from infinite to finite length scales

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Abstract: Hydrophobicity manifests itself in different forms across chemistry and physics, from solutes to surfaces, however, little is known about the unifying concepts behind these two interactions. A link between hydrophobicity on the infinite and finite scales would provide a more fundamental understanding of this interaction. This is difficult to achieve experimentally, and hence we aim to provide a thorough theoretical and computational study, through classical Density Functional Theory and Grand Canonical Monte Carlo simulations, of the processes underlying hydrophobic interactions. Previous studies have typically focussed on measuring the density profiles of water near substrates, however recently an alternative measure in the compressibility profile [1] has been suggested. Large fluctuations in the compressibility have been shown to be an indicator of hydrophobicity for a study of SPC/E water and a Lennard-Jones fluid, and we aim to utilise this measure to explore hydrophobic interactions of surfaces and solute particles. We aim to achieve this using a more realistic water model, monatomic water [2], and also to investigate whether a realistic water model is truly necessary, or, whether a simple Lennard-Jones fluid will suffice to capture the essential physics.

[1] Evans, R., and Wilding N.B. 2015. Quantifying Density Fluctuations in Water at a Hydrophobic Surface: Evidence for Critical Drying. *Phys. Rev. Lett.* **115** 016103.

[2] Molinero, V., and Moore, E. B. 2009. Water Modeled As an Intermediate Element between Carbon and Silicon. *J. Phys. Chem. B.* **113** 4008-16.