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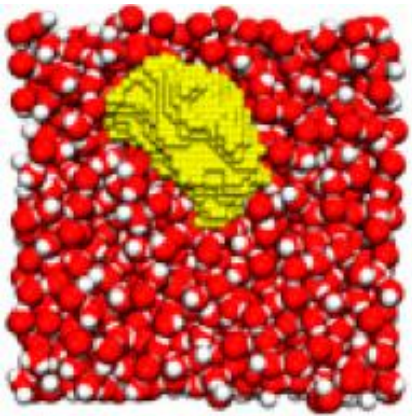
Cavitation in homologous liquids: experimental and theoretical study

The equilibrium between liquid and vapor, and between liquid and solid are archetypal phase transitions. Because of their first-order nature, the liquid state can persist beyond the equilibrium lines: the liquid can be stretched at negative pressure, or supercooled below the corresponding solid melting point. These states are metastable and the system will return to equilibrium through nucleation of the stable phase: nucleation of vapor or cavitation in the stretched liquid, crystallization in the supercooled region. These phenomena have important natural and technological consequence. For instance, the radiation balance of a cloud is different when the water it contains is a supercooled liquid or ice.

Our group has a long tradition of experiments on metastable liquids, and has developed several theoretical models to understand the experimental results.

The goal of the proposed internship is to systematically investigate cavitation in families of fluids, and interpret the results with a corresponding states analysis. Experimentally, cavitation will be triggered with n-alkanes by a focused ultrasonic wave. The cavitation pressure will be measured using a fiber-optic probe hydrophone [1,2]. Theoretically, we will study a family of interaction potentials. A first approach will involve density functional theory, which will be later complemented by molecular dynamics simulations.

A PhD can follow on various aspects of metastable liquids (at negative pressure, supercooled or supersaturated) or two-state models for metastable water [3,4], in collaboration with theorists (L. Joly in Lyon, groups of C. Valeriani in Madrid and M.A. Anisimov in Maryland).



Critical cavitation bubble inside water stretched at -150 MPa as obtained from molecular dynamics simulations combined with rare events sampling techniques [5].

[1] A. Arvenga, K. Davitt and F. Caupin, *Rev. Sci. Instr.* **82** 034904 (2011).
[2] N. Bruot and F. Caupin, *Phys. Rev. Lett.* **116** 056102 (2016).
[3] J.W. Biddle *et al.*, *J. Chem. Phys.* **146** 034502 (2017).
[4] P. Montero de Hijes *et al.*, *J. Chem. Phys.* **149** 094503 (2018).
[5] G. Menzl *et al.*, *PNAS* **113** 13582-13587 (2016).