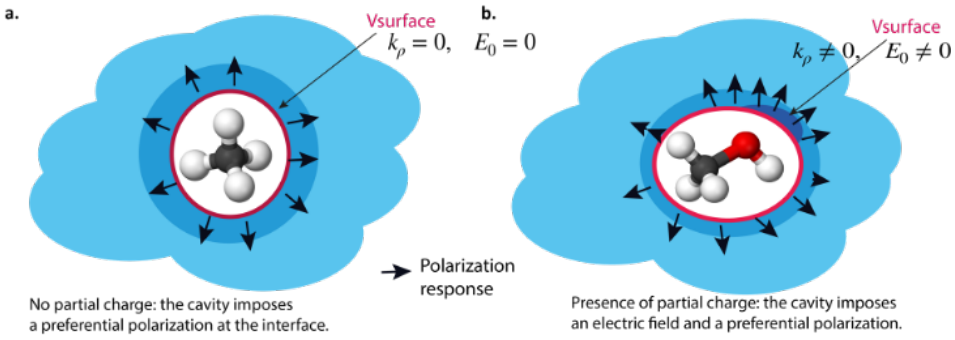
INTERNSHIP PROPOSAL

Laboratory name:Gulliver
CNRS identification code: UMR 7083
Internship director'surname: Hélène Berthoumieux
e-mail:helene.berthoumieux@espci.fr Phone number:
Web page: https://www.gulliver.espci.fr/?-people-
Internship location: ESPCI

Thesis possibility after internship: YES
Funding: NO If YES, which type of funding:

Fast computation of solvation energy for drug design.



Sketch illustrating the polarization induced in water by a solvated methane and methanol.

Solvation energy is a key quantity for drug discovery. The standard approach is to compute it using MD simulations, but this is time consuming for screening large numbers of molecules. We have developed an **implicit multiscale model for water**, where water is described as **coupled polarization modes across scales**. Unlike traditional approaches, density is excluded as non-essential information.
The polarization functional for water has already been validated for confined systems and hydration layers[1,2]. This internship will focus on **extending and applying the functional to compute solvation energies for molecules**, starting with simple molecules and progressing to those of pharmaceutical interest, in collaboration with the startup **Aqemia** [3]. The goal is to demonstrate the functional's **accuracy, efficiency, and relevance for drug discovery applications**

[1] J. G. Hedley, et al., J. Phys. Chem. 127, (2023)
[2] G. Monet, et al. Phys. Rev. Lett., 126 (2021)
[3] https://aqemia.com/science

Please, indicate which speciality(ies) seem(s) to be more adapted to the subject:

Condensed Matter Physics: YES/NO Soft Matter and Biological Physics: YES/NO
Quantum Physics: YES/NO Theoretical Physics: YES/NO