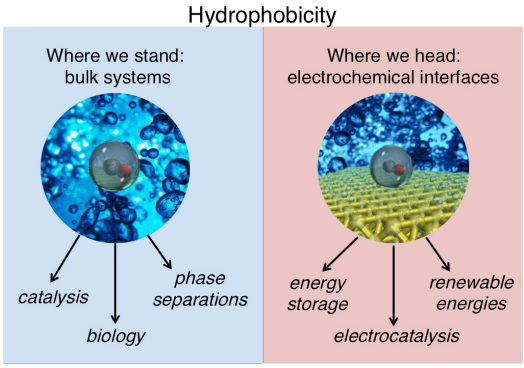
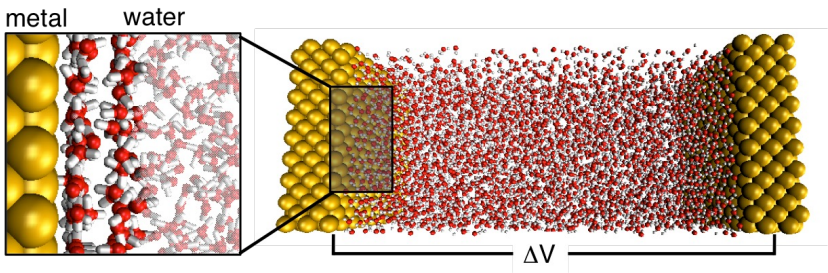
POST-DOCTORAL POSITION

Hydrophobicity and solvation properties at electrochemical interfaces from molecular dynamics and theory

The last two decades have seen an explosion of scientific interest in hydrophobic solvation due to its stunning importance for biology, catalysis and environmental science. However, it is only recently that we realized how important hydrophobicity is for electrochemical interfaces. There, hydrophobicity manifests in unexpected ways and hydrophobic molecules are involved in key electrochemical reactions, such as CO_2 reduction. Understanding and predicting hydrophobic solvation contributions to electrochemical reactions is expected to advance our comprehension, unlocking new ways to improve their efficiency. This can only be achieved through a substantial advance in theoretical understanding. The Lum-Chandler- Weeks theory[1] that revolutionized our comprehension of hydrophobic solvation does not hold true at electrochemical interfaces. The reasons are the unique combined effects of the layering of the aqueous electrolytes at the interface and the applied potential.

The successful candidate will use state-of-the-art constant potential molecular dynamic simulations to understand hydrophobicity and solvation properties of several electrified metal-aqueous interfaces. Then, the knowledge obtained from the simulations will be used to develop a new hydrophobic solvation theory for the interface. The gained knowledge will give us precious directions for how we can exploit hydrophobicity to regulate and improve many electrochemical processes.





1) K. Lum, D. Chandler, J.D. Weeks, Hydrophobicity at Small and Large Length Scales. *J. Phys. Chem. B* 103, 4570 (1999) .

2) A. Serva, M. Salanne, M. Havenith, S. Pezzotti, Size dependence of hydrophobic hydration at electrified gold/water interfaces. *Proc. Natl. Acad. Sci.* 118, e2023867118 (2021).

Period: 01/2024 – 01/2026. The position is funded by the Europen Research Council (ERC), grant num. 101077129.

Environment: The candidate will be hosted at the PASTEUR laboratory of the Chemistry Department of the Ecole Normale Supérieure in Paris. PASTEUR lab covers a broad range of physical chemistry and chemistry for life sciences. It offers a stimulating environment with 30 staff members, about 40 PhD students and 15 post-docs, in the center of Paris. We value people from different life experiences with a passion for research. The candidate will work together with myself and a PhD in my group. This position provides fundings for several national and international conferences in fields of interfaces and solvation that the candidate will have the chance to attend if interested.

Candidate profile: This position covers the most important part of my ERC project on hydrophobic solvation in electrochemistry. It will challenge the candidate to understand many fundamental aspects of physical and chemical properties of interfaces and solvation that remained poorly understood so far. Therefore, I am looking for candidates who are motivated to take on big challenges. The candidate will have the chance to contribute her/his own ideas and will have an important role in the initial development of my research group at the laboratory PASTEUR (ENS). Programming skills (c/c++, FORTRAN or python) and/or knowledge in the field of molecular modeling (molecular dynamics) are preferred. The candidate must have a PhD degree in Chemistry, Physics or Materials Science.

How to apply: To apply, please send us a CV, a short letter explaining why you would like to join us, your PhD certificate and one or two reference persons. The initial deadline for the application is Dec 1st, 2023.

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