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"Electric Fields At Aqueous Interfaces: Can They Drive Chemistry?"

In the last decade, there has been a surge of experiments showing that certain chemical reactions undergo an enormous boost when taken from bulk aqueous conditions to microdroplet environments. The microscopic basis of this phenomenon remains elusive and continues to be widely debated. One of the key driving forces invoked are the specific properties of the air-water interface including the presence of large electric fields and distinct solvation at the surface.

In this talk, I will take an atomistic dive into this problem with the goal of attempting to deconstruct the arguments that have been put forward to rationalize the apparent unique properties of the surface of water. My discussion will focus on three main topics highlighting mostly *negative results*:

- As part of a joint theoretical and experimental effort studying soap-bubble films for applications relevant for artificial photosynthesis, we found the presence of a highly polarized layer of water in a surfactant layer which generates a gigantic electric macroscopic electric field at the interfaces [1]. Experimental attempts to harness these electric fields to enhance reactivity have yet to be fulfilled.
- Through some judicious choices of modeling specific chemical reactions, including water autoionization [2] and Diels-Alder organic chemistry [3], we find that electric fields at interfaces do not result in any significant boost of catalysis.
- Finally, I will share some recent insights into the concepts of interfacial solvation and electric fields at the surface of water using phenol as a model system. Both the statics and dynamics of electric fields experienced by the phenol at the interface are not particularly different from those in bulk conditions. Combining our understanding of the chemical physics of solvation and an information theory based statistical test, we show that electric fields and solvation are inseparable quantities [4].

I will conclude with some perspectives on future directions that we are pursuing, specifically on photoinduced chemical reactions where electric fields may play a more prominent role.

[1] Gera et al., J. Am. Chem. Soc. 2021, 143, 37, 15103–15112.
[2] Di Pino et al., Angew. Chem. Int. Ed. 2023, 62, e202306526.
[3] Gong et al., J. Am. Chem. Soc. 2024, 146, 46, 31585–31596.
[4] Di Pino et al., https://doi.org/10.48550/arXiv.2506.23988.