

Molecular dynamics modelling of electrode-electrolyte interfaces

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Abstract: The potential of an electrode is the difference in electrostatic potential between the conducting solid and electrolyte. It is not a work function and cannot be directly measured. Experimental electrochemistry resolves this issue by measuring the potential of a “working” electrode relative to a reversible reference electrode. The potential across the interface of the reference electrode with the electrolyte is held fixed by a fully reversible electrode reaction. Such an ideal Faradaic electrode is practically impossible to construct in an atomistic simulation. After reiterating this important point, which is not always fully appreciated, I briefly review our attempts to address this difficulty applying finite electric field techniques to a periodic molecular dynamics cell containing a single slab of electrode and electrolyte (all treated classically at this stage). This method enables us to compute and control the *sum* of the electrode potentials across the two interfaces of the conducting slab. This work is in collaboration with the group of Mathieu Salanne (Sorbonne, Paris)[1,2].

References:

- [1] T Dufils, G Jeanmairet, B Rotenberg, M Sprik, M Salanne, *Phys. Rev. Lett.*, **2019**, *123*, 195501
- [2] T Dufils, M Sprik, M Salanne, *J. Phys. Chem. Lett.*, **2021** (*in press*)
- [3] JQ Li, L Meng, M Sprik, J Cheng, *J. Chem. Phys. C.*, **2020**, *124*, 19003
- [4] M Sprik, *Phys. Rev. E.*, **2021**, *103*, 022803



Biography: After a long period of work in computational electrochemistry using electronic structure calculation based molecular dynamics methods (mostly in collaboration with Jung Cheng, see Ref. [3]) I have turned in my more recent research to classical molecular dynamics [1,2] and even continuum theory [4] aiming to investigate the electromechanics of electrochemical interfaces.