A3-06 Characterizing the electrolyte/graphene interface: an integrated approach with modelling and experiments

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The physical-chemistry of the graphene/aqueous–electrolyte interface underpins the operational conditions of a wide range of devices. Despite its importance, this interface is poorly understood due to the challenges faced in its experimental characterization and the difficulty of developing models that encompass its full physics. [1]
In this talk I'll show how combining molecular simulations with experiments, it is possible to investigate the relationship between wetting, double layer structure, friction coefficient and interfacial dynamics and understand how these properties are related to the capacitive properties of the interface. I'll initially introduce the new multiscale modelling techniques we developed to capture the ions-induced polarization of graphite modelling simultaneously the coupled motion of the surface electrons and ions in the solution.[2, 3] Then I'll show some application of the methods to electrified bulk interfaces and under confinement and show how the simulation results can be an invaluable tool to understand experimental data.[4, 5]

1）J. D. Elliott, A. A. Papaderakis, R. A. W. Dryfe, P. Carbone, *J. Mater. Chem. C*, **2022**, *10*, 15225.
2) J. D. Elliott, A. Troisi, P. Carbone, *J. Chem. Theory Sim*., **2020**, *16*, 5253.
3) N. DiPasquale, J. D. Elliott, P. Hadjidoukas, P. Carbone, *J. Chem. Theory Sim*., **2021**, *17*, 4477.
4) J. D. Elliott, M. Chiricotto, A. Troisi, P. Carbone, *Carbon*, **2023**, 292.
5) Z. Wei, J. D. Elliott, A. A. Papaderakis, R. A. Dryfe, P. Carbone, *J. Am. Chem. Soc*., **2023**, *146*, 760.

PROFILE

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Paola Carbone is Professor of Computational and Theoretical Chemistry in the Department of Chemistry of the University of Manchester and currently chair of the CCP5. She obtained her PhD in Material Science from "Universita' Bicocca" in Milan (Italy) in 2004. After a 2-years postdoc at the University of Bologna, in 2006 she was awarded a fellowship from the Humboldt Foundation and joined the group of Prof. Mueller-Plathe in Darmstadt (Germany). In 2008 she moved to the University of Manchester with a RCUK fellowship where she is now Professor in Computational and Theoretical Chemistry. Her area of expertise is simulations of soft matter and her group specializes in developing new multiscale coupling procedures to link different modelling techniques from quantum mechanics to dissipative particle dynamics. Currently active research areas are: electrolyte/graphene interfaces, polymer composites for industrial applications and surfactant solutions.