Università degli Studi di Milano Bicocca
Dipartimento di Scienza dei Materiali
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Seminar room – Department of Materials Science U5

Multi-scale modeling framework for complex processes at heterogeneous functional interfaces

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Great research efforts are currently devoted to design and development of energy conversion and storage technologies: batteries, photo-electrochemical cells, perovskite solar cells, fuel and electrolyzer cells are some examples. From a general perspective, these different devices share a common functioning principle that is based on charge and mass transport across several layers of materials and functional interfaces. Several crucial issues related to these devices and their constituent materials are still open. In particular, the heterogeneous interfaces are the locus of key physico-chemical processes that affect the most the overall conversion/storage performances. Computational investigations can be pivotal in dissecting the subtle structure-property-function relationships in these complex interfaces and their constituent materials. However, the standard first-principles approaches are often too idealized to describe these devices in operating conditions. The main problem is the lack of a unique theoretical approach able to tackle, at the same time, all the effects that tune the interface reactivity and chemistry. This calls for new computational strategies. In this context, this talk will address some case studies highlighting the challenges in modeling energy-related technologies and the most suitable ab-initio approaches to account external variables, including solvent dynamics [1], applied electric bias [2], and chemical reactivity at strongly correlated interfaces [3,4]. The results will point out the need of building a new multi-scale paradigm bridging different time and space scales for modeling electrochemical devices by means a bottom-up perspective based on quantum mechanics.

[1] Fasulo, F.; Piccini, G.M.; Muñoz-García, A. B.; Pavone, M.; Parrinello, M; *J. Phys. Chem. C* **2022**, *126*, 15752-15758
[2] Fasulo, F.; Massaro, A.; Muñoz-García, A. B.; Pavone, M. *J. Mater. Research* **2022**, *37*, 3216–3226
[3] Fasulo, F.; Massaro, A.; Muñoz-García, A. B.; Pavone, M.; *manuscript under review*
[4] Fasulo, F.; Muñoz-García, A.B.; Massaro, A.; Crescenzi, O.; Huang, C.; Pavone, M., *J. Mater. Chem. A* **2023**, *11*, 5660-5669