DIPARTIMENTO DI FISICA E ASTRONOMIA "ETTORE MAJORANA"

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Theory meets experiments to uncover the reaction mechanisms at electrochemical interfaces

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Abstract

Electrochemical energy conversion and storage processes, such as water splitting and Li-ion intercalation in batteries, rely on complex interfacial reactions that govern both efficiency and stability. At these interfaces, activity and stability are often closely linked because they are controlled by the same material properties, making it necessary to balance the two when identifying optimal materials for these applications. Understanding the underlying reaction mechanisms at the atomic level is essential for designing sustainable and long-lasting electrochemical interfaces with improved activity. However, electrochemical interfaces are difficult to probe because of their limited accessibility and the complexity of the phenomena occurring simultaneously.

This talk will show how first-principles calculations, combined with experimental techniques, can unambiguously reveal the reaction mechanisms of interfacial electrochemical processes. We will illustrate how this combined approach enabled the discovery of unconventional reaction mechanisms in oxygen evolution electrocatalysis on oxides. In a second example, we will discuss how the chemical reactivity at the oxide-electrolyte interface in Li-ion batteries strongly depends on the oxide composition, identifying design strategies to prevent parasitic reactions. These results highlight the critical role of the oxide electronic structure, and particularly the position of the oxygen states, in determining surface reactivity and, consequently, electrochemical performance.

[1] A. Grimaud et al., "Activating lattice oxygen redox reactions in metal oxides to catalyze oxygen evolution" Nat. Chem. 9, 457 (2017).

[2] R. R. Rao et al., "Operando Identification of Site-Dependent Water Oxidation Activity on Ruthenium Dioxide Single-Crystal Surfaces" Nat. Catal. 3, 516 (2020).

[3] G. Di Liberto, et al., "Role of Water Solvation on the Key Intermediates Catalyzing Oxygen Evolution on RuO2" J. Phys. Chem. C 127, 10127 (2023).

[4] Y. Zhang, et al. "Revealing electrolyte oxidation via carbonate dehydrogenation on Ni-based oxides in Li-ion batteries by in situ Fourier transform infrared spectroscopy" En. Envir. Sci. 13, 183 (2020).

[5] L. Giordano et al. "Molecular trends in the C-H oxidation of organic molecules on oxide surfaces: implications for electrolyte reactivity at the positive electrode in Li-ion batteries", in preparation.

Livia Giordano is a Full Professor at the University of Milano-Bicocca. From 2013-2021 she worked at the Massachusetts Institute of Technology, where she led the computational chemistry research in the Electrochemical Energy Laboratory at the Department of Mechanical Engineering, and from 2019 to 2021 she served as program manager of the Low Carbon Energy Center for Energy Storage for the MIT Energy Initiative. She earned her PhD in Material Science from the University of Milano-Bicocca and joined its faculty in 2007. Her research combines mechanistic understanding and reactivity trends to design materials for energy storage and conversion, with emphasis on electrode–electrolyte interfaces in Li ion batteries, novel electrolytes, and oxygen electrocatalysis. Her work has contributed to the discovery of new electrolytes for Li–air batteries and to the development of catalysts for the oxygen evolution reaction.

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