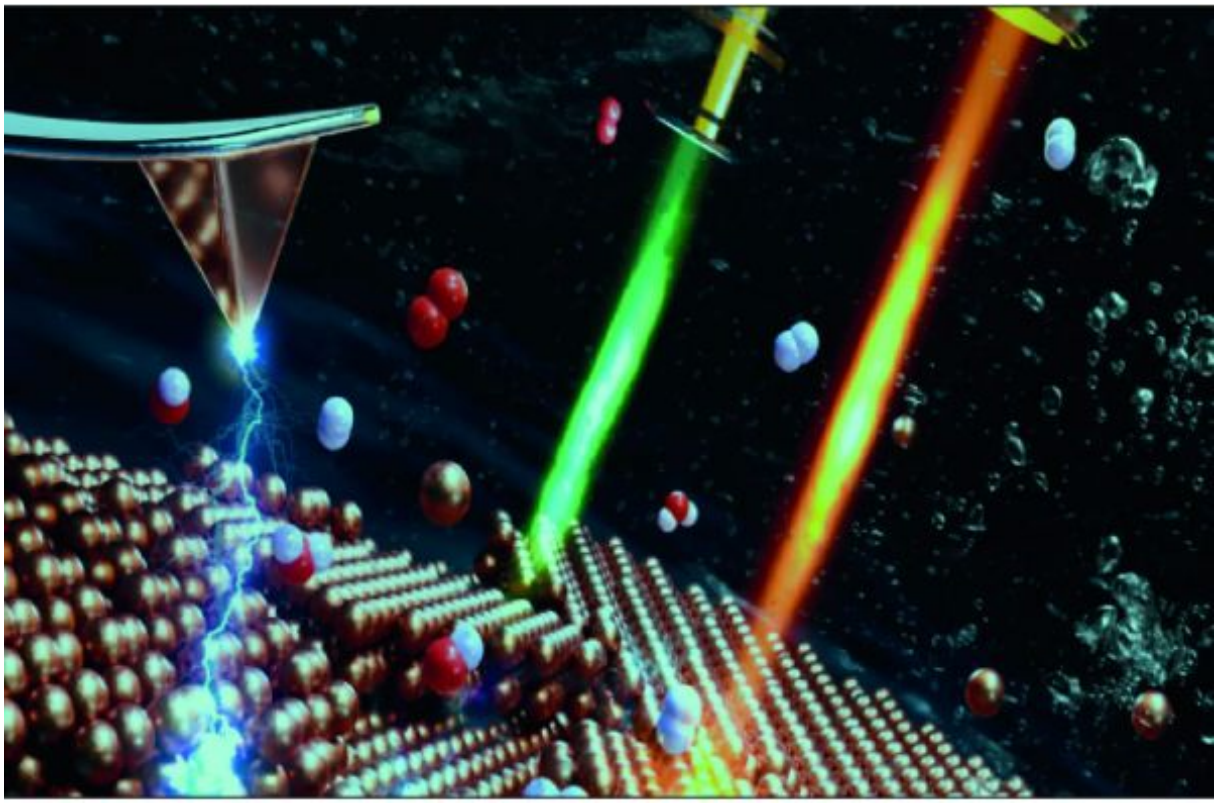


A holistic approach to enhance electrochemical interface studies

A new review published in Nature Reviews Chemistry discusses o how the combination of photonic, electronic, chemical, an mechanical probes can help shed light on so far unresolve aspects of electrochemical interfaces (EIs), one of the underlyin principles of energy conversion and storage.

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The electrochemical interface - typically comprising the junction between a polarized surface, a liquid (electrolyte), and dissolved reactants - is at the core of several manufacturing and energy storage technologies. These span from mature, well-established processes, such as the chloralkali electrolysis, to batteries, fuel cells, and water electrolysis for the production of solar fuels.

EIs drive the atomic and molecular transformations that determine the performance in these devices. However, its predictive design - needed to enable further performance advances - is challenged by its highly dynamic character, which comes hand-in-hand. EIs can drastically change during operation, from intrinsic dynamic changes related to electron and energy

transfer, and the supported reactions; to extensive surface reconstruction, including changes in electronic configuration and structure.
Assessing EIs at relevant working conditions (typically referred to as in situ and operando, depending on how close the conditions are to actual operation) is thus crucial to understand those principles that govern the reactions occurring at the interface and to enable its informed design.
Traditionally, EIs have been studied applying different methods that could probe some specific aspect (e.g., either structure or composition) with a given resolution, only providing partial, incomplete insights of these interfaces.
In this context, **Dr. Lu Xia and ICFO Prof. Dr. F. Pelayo Garcia**, together with former ICFOnian Dr. Ernest Pastor, lead a multidisciplinary consortium that reviews the prospects of combining different photonic, electronic, chemical, and mechanical probes, to offer a more complete view of these EIs. The review, published in Nature reviews chemistry, highlights the opportunities of such combinations to overcome traditional spectroscopic limitations and to bridge the existing gap between theoretical modeling, ideal systems, and working interfaces - ultimately enabling the predictive design of EIs and devices with improved performance.

From individual techniques to a complementary and theoretical approach
The study starts by acknowledging the individual analytical techniques that have been used in the past to probe electrolysis devices. It describes the properties each of them can retrieve, their advantages as well as their drawbacks. As it has been suggested before, there is a common inconvenient to all of them: each approach can only grant access to a limited set of properties of the EI, providing just a partial picture of the whole mechanism.
In fact, EIs are highly heterogeneous, intricated and dynamic, which makes single-method studies insufficient to grasp the EI in all its complexity. Within the review, the researchers acknowledge the power of mixing independent approaches to better resolve different properties of the EI and to prevent misleading interpretations which may not be detected by a single probe.
i¿½Recognizing the current fragmented research efforts -often isolated within specif c methodological approaches- we aimed to bridge these divides by showcasing the power f combining various analytical techniques and theoretical insights. This strategy is aimed t fostering cross-disciplinary collaboration and innovation in the fieldi¿½, explains Lu ia. According to the author, addressing the complexity of the EI in a holistic manne by combining multiple techniques (simultaneously or sequentially) and being theoretic lly informed is essential for the development of this fi ld. The review gives a long list of complementary approaches and details for their are of activity. For example, combining Electrochemical Impedance Spectroscopy with Sur ace Enhanced Raman Spectroscopy (two experimental methodologies usually applied separat ly) and integrating them with Density Functional Theory simulations (a theoretical descriptio

of the EI) can unlock a better understanding of several processes (charge transfer and chem cal transformations) taking place at the interface. It can also predict the formatio of intermediate species (transient elements that form along an electrochemical reaction), w ich can point out why certain interactions proceed efficiently or not. With these characteris ics being revealed, a deeper knowledge of reaction mechanisms in EIs is possi le. In the near future, their work can be used by other scientists to develop, optimize and g ide the design of a wide range of electrochemical technologies, including fuel cells, batter es, electrolysers for hydrogen production and CO_2 electrochemical reduction systems. To do so, new experimental set-ups based on their complementarity principle need to be standardized. If implemented, this procedure could enable a broader base of researchers to contribute to this field. So far, the team has already provided a reference point that will help them to identify useful, complementary methods, suitable for probing EIs in action.

Bibliographic reference

Pastor, E., Lian, Z., Xia, L. et al. Complementary probes for the electrochemical interface. Nat Rev Chem (2024). https://doi.org/10.1038/s41570-024-00575-5

Caption: Illustration of complementary photonic, electronic, chemical, and mechanical probes in unraveling the complex mechanisms at electrochemical interfaces (EI), including bonding, intermediates and the transformation of reactants at the molecular or atomic level.