What can we learn about energy conversion from quantum mechanics?

Francesca Fasulo[1], Ana B. Muñoz-García[1], Michele Pavone[2]

[1]Department of Physics "E. Pancini", University of Naples Federico II, Napoli, 80126, Italy
[2]Department of Chemical Sciences, University of Naples Federico II, Napoli, 80126, Italy

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Advances in energy technologies, such as batteries, photoelectrochemical cells and solar cells, have highlighted the critical role of heterogeneous interfaces in determining device performance and stability. Despite significant progresses, many challenges remain unsolved due to the subtle physical and chemical processes at these interfaces [1]. The complexity of interfacial chemistry often requires computational investigations to provide valuable insights into reactivity, structural and electronic behavior of constituent materials, and to optimize the design of the most suitable ones [2-6]. Nevertheless, the computational study of such complex systems is not straightforward and a reliable description of each occurring phenomenon is not feasible within a unique framework. An in-depth understanding of interface reactivity and chemistry calls for new strategies beyond the standard computational approach. In this context, here we present applications of embedded cluster multireference calculations [7] to elucidate how surface Ir-oxo species contribute to efficient oxygen evolution reactions (OER) [8]. The complexity of electronic correlation effects in molecular reactivity at electrode interfaces often requires multireference approaches beyond the Density Functional Theory (DFT). This study highlights that embedded methods can offer a more accurate description of molecular reactivity and energy barriers at electrode interfaces [8-10]. Overall, we demonstrate how first-principles investigations can gain valuable insights into designing effective catalysts and into advancing knowledge on reactivity at the complex heterogenous interfaces in energy devices, paving the way for future innovations in sustainable energy technologies.

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