Quantum chemical design of multi-component perovskite oxides for energy conversion devices

Michele Pavone

Dipartimento di Scienze Chimiche, Università di Napoli Federico II, Via Cintia 21, 80126 Napoli, Italia michele.pavone@unina.it

Global advances in industrialization are precipitating the rapid consumption of fossil fuel resources with increasing levels of atmospheric greenhouse gases. After the UN international conference on climate change (Paris 2015) and despite the recent political shift in USA, there is a worldwide consensus on implementing all possible actions to dislodge our dependence on oil, coal and natural gas. World sustainability requires viable sources of renewable energy and new technologies for its efficient conversion into commodities such as fuels or electricity.

Material Sciences play a pivotal role in optimizing the functional materials that are at the core of energy conversion devices. This is not a trivial task. The conversion of energy is the result of several physical and chemical processes that involve chemical reactions, charge and mass transport occurring across heterogeneous interfaces. Often, experimental techniques cannot dissect subtle features at the nanoscale that can hinder an effective design of new devices. Thus, the application of computational modeling tools with atomistic resolution represents an ongoing revolution in materials design and device development.

In this context, Quantum Mechanics (QM) offers an unbiased guide for characterizing the complex materials properties and predicting the key processes at the atomic scale. In particular, I will review our recent QM studies of electrode materials for energy conversion devices, with a specific focus on solid oxide electrochemical cells [1-4]. Our results will highlight the merits of Density Functional Theory for gaining qualitative insights on important materials properties. At the same time, we will discuss the limits of current standard approaches for complex reactions at heterogeneous interfaces, as for example the oxygen reduction reaction at electrode surfaces. Last but not least, the future directions for the application of quantum chemistry to renewable energy technologies will be outlined.

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