Charge and electron transfer in energy related devices

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Although most of the technologies underpinning renewable energies are (in principle) ready for large-scale implementation, they still require improvement in order to be competitive at both efficiency and economical level with more traditional sources. Design, synthesis, characterization and application of new materials represent a long process often involving several experimental steps each of them requiring significant human and financial resources. Computational materials science can support and speed up this process. Indeed the understanding of microscopic chemical processes at the base of the energy production can provide valuable insights for their improvement. To this end, an effective computational protocol rests on an expert combination of different ingredients, including a reliable approach for electronic structure, an effective model for environmental effects and an interpretation scheme able to covert quantum chemical results in simple yet valuable chemical concepts. This philosophy will be illustrated with selected examples concerning the analysis of charge and electron transfer or transport in some energy-related devices, such as solar and fuel cells.