Characterization of photoelectrochemical processes for energy conversion through computer simulations

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In this talk, I will show how computer simulations based on first principles can provide insight into crucial processes for energy conversion taking place at the photoelectrode and at the interface between photoelectrode and electrolyte in photoelectrochemical cells. Relations between atomic structure of the system and photoabsorption, charge transfer, and chemical reactivity are investigated, and lead to a deeper understanding of the functional behaviour of the materials. These results help the interpretation of electrochemical measurements, and may guide the development of better photoelectrodes.