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Title: Harvesting solar energy: DFT studies of organic photovoltaics and photo-catalytic water splitting

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Then sun is the largest provider of renewable energy in the solar system. Yet, so far directly harvesting solar energy constitutes only a small part of the world's energy supply even compared to other renewable energy sources. In our contribution we will discuss our theoretical research on two promising methods which could change this. First, organic solar cells, which are envisaged as a promising alternative to silicon based solar cells. They are cheap and easy to produce, light and flexible, and easily deployed on walls or roofs. Unfortunately, these advantages currently come at the price of small photo-electric conversion efficiencies. One of the loss mechanisms is inefficient charge transfer in the semiconducting layers. To gain atomistic insight into this process, we used advanced density functional theory (DFT) based methods to investigate the electron-conducting properties of modified fullerene crystals, which form in the nano-crystalline domains of the n-type semiconducting layer in organic solar cells. Based on the DFT results we employed a kinetic Monte Carlo (kMC) model which allowed us to predict macroscopic electron mobilities, which are also accessible to experiments. Second, we will discuss our ongoing efforts in the field of photo-catalytic hydrogen production. Molecular hydrogen is a promising alternative to batteries when it comes to energy storage in that it can, in highly compressed liquid form, provide much higher energy densities than all current battery designs. We will report on our DFT based research on photo-catalytic water splitting on titanium dioxide semiconductors, nano-patterned with small (3-20 atom) gold nano-clusters. We investigate the suitability of these clusters as co-catalysts for the water oxidation reaction and identify trends with respect to cluster size. The aim of these efforts is to understand the mechanisms involved and their dependence on system structure, enabling th design of high yield catalysts.