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Probing Nanointerfaces of Nanoparticle-Based Solar Energy Conversion: Molecular Dynamics on the Angstrom Scale[1]

RICHARD OSGOOD[2], Columbia University, Laboratory for Light-Surface Interactions, Center for Integrated Science and Engineering

Charge-induced surface chemistry following solar-illumination of nanometer-scale semiconductor particles is one possible route to low-cost solar energy conversion. Because of their high surface to volume ration interfaces play a major role in the performance of this technology and thus the physics of charges interacting with adsorbed molecules is of central interest. In this talk, after a brief review of related work, we will focus on our advances in understanding molecular-dissociation-dynamics at the interface of nanometer-scale TiO_2 crystals and large organic molecules. Clearly the standard probes of beam-based molecule dynamics are not easily adaptable to small nanointerfaces. Instead our work uses STM imaging to examine dynamics of fragments following tip-induced electron injection into organic molecules on TiO_2 (110) and on $\sim$10nm nanocrystals (110). Our experiments have used halogenated anthracene to probe the efficiency and fragment trajectory following dissociative electron capture. Our work has examined nanoparticle synthesis, adsorbate-molecule orientation, thermal and injected-electron chemistry, and adsorbate charge-mediated fragmentation trajectories.

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[2]Second author: Denis Potapenko