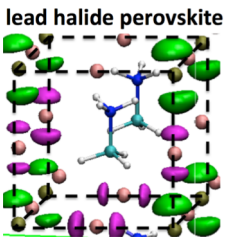
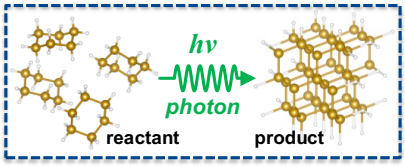
256th ACS National Meeting & Exposition
Nanoscience, Nanotechnology & Beyond
August 19-23, 2018 | Boston, MA
ACS COMP Symposium

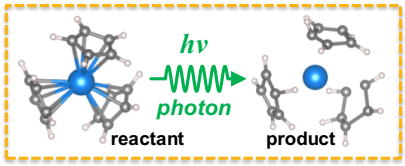
Computational Photocatalysis: Modeling of Photophysics & Photochemistry at Interfaces

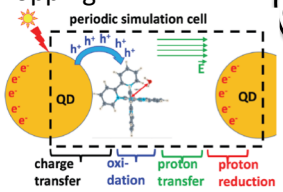
The study of photochemical reactions in general and photoelectrochemical water splitting in particular, rests on understanding of such elementary effects as light absorption, energy transfer, electron transfer, radiative and nonradiative relaxation, and catalysis is important for the rational design of efficient system for energy conversion. The design of most efficient catalysts is pursued by change of composition, quantum confinement, size, shape, surface functionalization, magnetic doping, and mesoscale structural arrangement providing versatile tuning of timescales of available basic mechanisms and properties of materials. This symposium presents recent experimental and computational synergistic advances on modeling of photophysics and photochemistry at interfaces: Experimental achievements stimulate further development of more precise theoretical methods. Computational modeling allows for interpretation of available experimental trends and help in guiding further advances in design of efficient photocatalytic materials It is expected that the symposium will bring better understanding of photoinduced processes of light absorption, formation and breaking of charge transfer excitations, hot carrier relaxation, and redox reaction dynamics at catalytic sites – affected by lattice vibrations and solvent polarization.

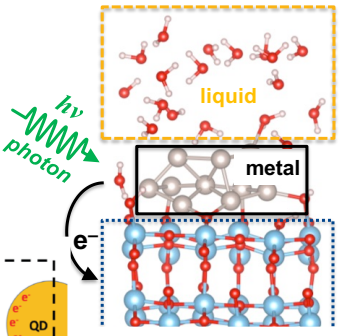


- ❑ Novel Materials for Photocatalysis
- ❑ Reactions of reactants adsorbed to catalytic sites
- ❑ Photoexcitation role in Reaction Pathway
- ❑ Quantum nature of reactions: proton coupled electron transfer
- ❑ Charge transfer at interfaces
- ❑ Electronic relaxation: density matrix vs. surface hopping









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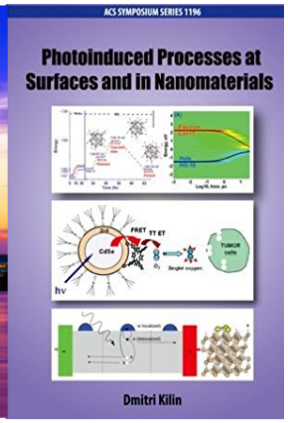
Submission Deadline: March 26, 2018

Abstract Submission: https://callforpapers.acs.org/boston2018/COMP

Proceedings published as ACS Book

Boston, Massachusetts August 19-23, 2018



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