Interfacial Electronic Properties in Oxide-Polymer Nanocomposites

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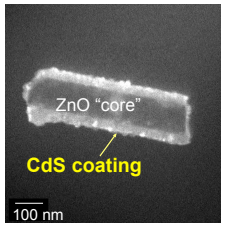
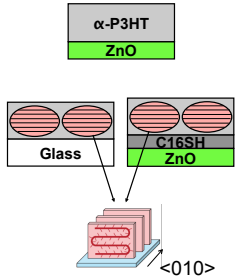
SAND2010-2053P

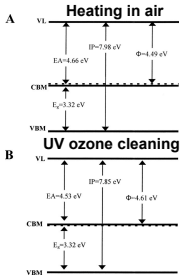


• *Background:* Understanding electronic structure at the organic-inorganic interface is critical to use these nanocomposites in sensing, energy harvesting and storage.
• *Goals:* Develop (1) a fundamental understanding of interfacial electronic properties, (2) interfacial modifications to enhance the desired optoelectronic properties of the nanocomposites, and (3) novel measurement techniques to probe buried interfaces of relevance.
• *Major results & significance:* Polymer-substrate interaction dramatically modifies the morphology of the polymer and affects interfacial charge recombination. Judicious interfacial modification and oxide engineering lead to improvement in photoresponse behavior in organic-inorganic nanocomposites.

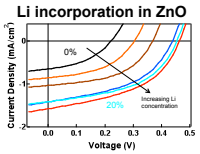


Research Description

- In collaboration with T. Kuech's group at U. Wisconsin, we applied photoelectron spectrscopies (PES) to probe how the electronic structure of ZnO surface depends on crystallographic direction and chemical processing.



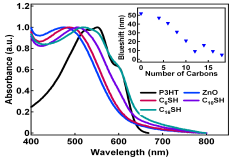
- Develop approaches, e.g. chemical doping and conformal coating, to modify the electronic and surface chemical properties of the ZnO electron acceptor so to improve interfacial polymer morphology and to optimize interfacial band alignment to facilitate electron transfer.

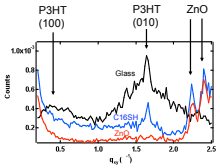


- Using grazing incidence X-ray diffraction and UV-vis spectroscopy to probe the ordering of polythiophene (P3HT) on oxide surface with organic/inorganic modification.
- Apply femtosecond transient absorption (CINT user project) to probe lifetimes of photoexcited species.

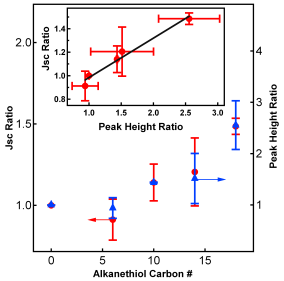
Major Results & Impact

- Strong interaction between ZnO and P3HT results in an undesired amorphous P3HT layer at the interface, leading to reduced overlap with the solar spectrum, shorter exciton lifetime, and lower photocurrent.

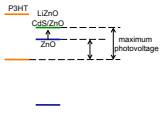




- The P3HT ordering is drastically improved with an alkanethiol monolayer at the heterojunction interface. The enhancement in photocurrent is shown to directly correlate with P3HT ordering. Exciton lifetime is measurably longer in ordered polymer layers.



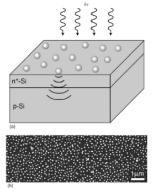
- Selective deposition of CdS nanocrystals on ZnO surface or incorporating Li in ZnO increase the energy offset between photoexcited electrons and holes and lead to higher photovoltage.



- Structural and chemical changes at the heterojunction interface are critically linked to carrier dynamics and optoelectronic properties of the nanocomposites and must be better understood in order to advance applications using these complex materials.

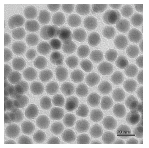
Future (@ UT-Dallas)

- It has been shown that surface plasmon effects of metal nanoparticles enhance absorption in solar cells. However, pure metal nanopartcles need to be insulated to prevent electrically shorting and quenching.

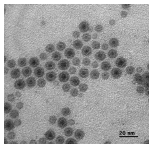


P. Matheu, APL 93, 113108 (2008)

- Based on Huber's previous work on controlled synthesis of Fe/FeO_x nanoparticles through surfactant engineering, other metal/dielectric core/shell nanoparticles will be explored.

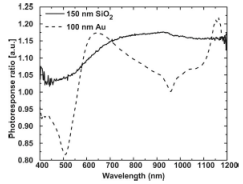


Large metal particle with thin oxide (l), Small metal particle with thick oxide (r).



- At UTD, Hsu's group will perform optical and electrical characterization of metal/dielectric core/shell nanoparticles made at Sandia for their applications in energy harvesting.

Photocurrent enhancement over device without nanoparticles



D. Derkacs, APL 93, 091107 (2008)

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000

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