BES016 Center for Interface Science: Solar-Electric Materials (CISSEM)

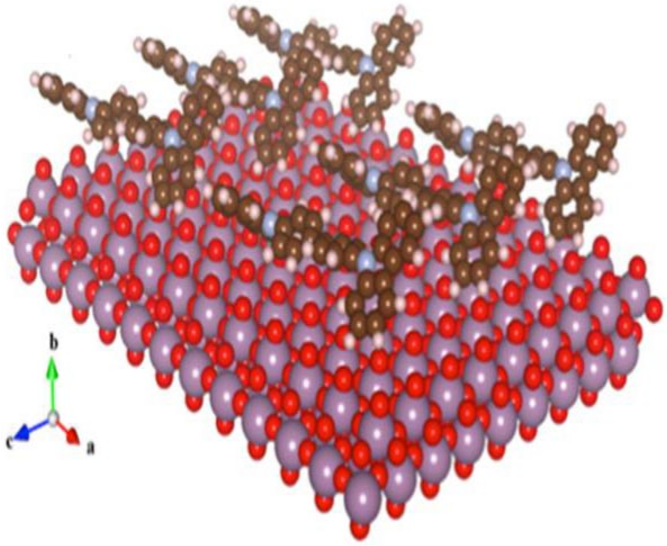
Presenter: Scott Saavedra
University of Arizona

Abstract

CISSEM was established on August 1, 2009 as an EFRC funded by the U.S. DOE, Office of Science, Basic Energy Sciences, under Award Number DE-SC0001084. We combine research groups at The University of Arizona (the lead institution), Georgia Institute of Technology, Princeton University, the University of Washington and NREL in a coordinated and integrated multi-investigator program. CISSEM's mission is to advance the understanding of interface science underlying solar energy conversion technologies based on organic and organic-inorganic hybrid materials; and to inspire, recruit and train future scientists and leaders in the basic science of solar electric energy conversion.

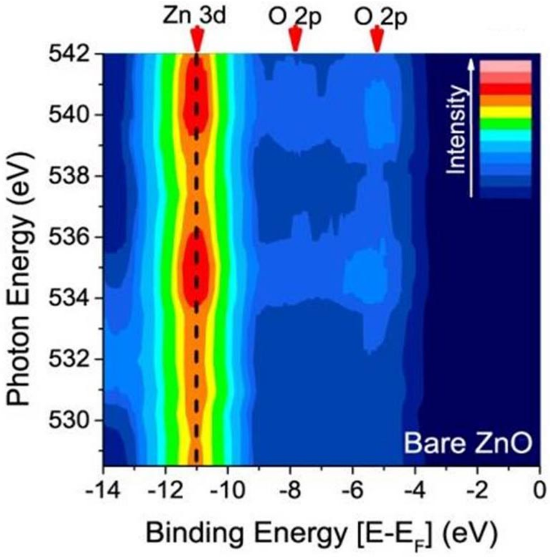
Continued improvement of thin-film photovoltaic (PV) energy conversion technologies –underpinned by basic science – is an exciting challenge that engages CISSEM. For "printable" solar cells based on hybrids of polymers, small molecules and semiconductor nanocrystals, the open-circuit photovoltage is limited by: *i)* the work function difference between two contacts, which is affected by the composition, structure and energetics at both contact/active layer interfaces; *ii)* the competition between charge harvesting and charge recombination, both in the active layer itself, and at the interfaces between electrical contacts and active layer components; and *iii)* other detrimental processes such as charge back injection from the contacts. By incorporating thin *interlayers* of appropriate inorganic or organic materials between each contact and the active layer, we can increase device efficiency by providing thermodynamic and/or kinetic barriers to help facilitate the desired preferential or 'selective' charge harvesting of either electrons or holes at each contact, while also minimizing charge back injection.

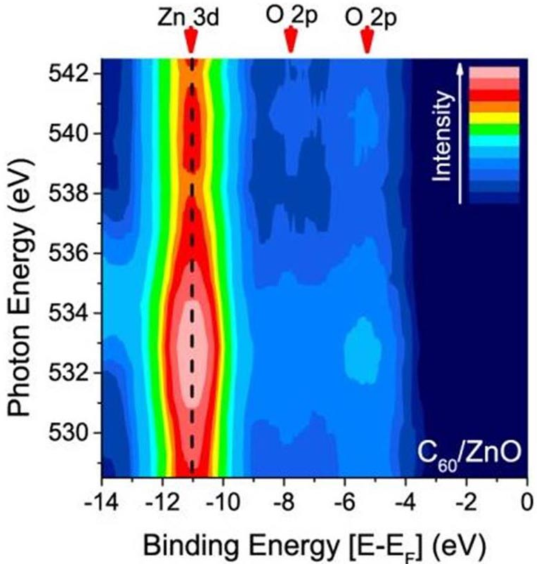
This poster highlights our experimental and theoretical research focused on understanding the principles of efficient charge harvesting, and providing a molecule/atomic scale understanding of how interface composition, structure, energetics and rates of charge extraction versus recombination control PV efficiency, i.e., through better contact and interlayer design and more efficient charge extraction. CISSEM research should ultimately provide design principles to help create a wide array of new energy conversion platforms, including the new perovskite-based PV platform, and the scientific foundations for thin-film PV technologies and our nation's pursuit of lowering costs to transform the sun's energy into electricity.



Above: Theoretical modeling of the organic hole-transport layer 4,4′-N,N′-dicarbazole-biphenyl physisorbed on the important, transition metal oxide surface MoO3 (010) – part of a combined theoretical and experimental study of facile hole collection and injection. [DOI: 10.1002/adfm.201301466]

Next Page: Using photoemission spectroscopy at SLAC to investigate the electronic structure and carrier dynamics at a model zinc oxide/fullerene (C_{60}) interface, like those used to selectively harvest electron in OPV platforms. Hybrid interface states form in both the ground and excited state manifold. Using resonant photoemission spectroscopy, we are able to observe ultrafast carrier delocalization in bare ZnO, with electrons scattering into bulk states on the time-scale of less than 500 as. In the presence of C_{60} (and hybridization between C_{60} and ZnO), the resulting interface state formation leads to carrier localization and long-lived excited states in the vicinity of the conduction band minimum. [*manuscript submitted*]


Zn 3d
O 2p
O 2p
542
540
538
536
534
532
530
Photon Energy (eV)
Intensity
Bare ZnO
-14
-12
-10
-8
-6
-4
-2
0
Binding Energy [E-E$_F$] (eV)


Zn 3d
O 2p
O 2p
542
540
538
536
534
532
530
Photon Energy (eV)
Intensity
C$_{60}$/ZnO
-14
-12
-10
-8
-6
-4
-2
0
Binding Energy [E-E$_F$] (eV)