Small molecule, polymer and perovskite photovoltaic cells with very high performance

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Solution-processed organic solar cells and organic-inorganic hybrid solar cells are among the most promising photovoltaic technologies for eventuallow-cost manufacture. In this presentation, I will briefly report our recent work towards realizing the potential of small molecule, polymer and perovskite photovoltaics.

(1) Small molecule OPV. Small molecule organic semiconductors have attracted increasing interest due to the advantages of its well-defined structures, facile synthesis and purification, and generally high charge carrier mobility. In the first part of my presentation, I will report high performance single junction and double junction OPV device based on DOR3T-BDTT. Using the solution spin-coating fabrication process, the certified power conversion efficiency (PCE) of 8.02% from single junction device was obtained. A homo-tandem solar cell was constructed with a novel solution processed interlayer (or tunnel junction), demonstrating an unprecedented PCE of 10.1%.

(2) The second part of my presentation is on polymer solar cells. Recently, we demonstrated two families of NIR conjugated polymers (Eg ~ 1.4 eV) specifically suitable for the tandem structure. One is based on alternating benzodithiophene/diketopyrrolopyrrole units and the other is based on alternating dithienopyran/diflourobenzothiadiazole units. In the single-layer devices, power conversion efficiencies (PCE) of 7~8% were achieved. When the polymers were applied to tandem solar cells, we demonstrated PCE of 10.6% (under the AM 1.5G solar condition). Furthermore, the tandem devices show excellent stability due both to the intrinsic stability of the polymer and the advanced device structure.

(3) The third part of my presentation is on the organic-inorganic hybrid perovskite based solar cells, particularly CH3NH3PbX3 (X=Cl, Br, I). We demonstrate a novel low temperature vapor assisted solution process to fabricate organic-inorganic hybrid perovskite films (e.g. CH3NH3PbX3, X=Cl, Br, I) and the corresponding photovoltaic devices. The perovskite films derived from this approach exhibit superior film quality, with full surface coverage, uniform grain structure with grain sizes up to the micron scale, and a complete precursor transformation. Facilitated by the excellent film quality, the CH3NH3PbI3 materials enable a PCE over 12% in a planar architecture. We have further improved device engineering, and our latest perovksite solar cell has reached efficiencies in the range of 15-18%*. We believe that further research in film formation, device architecture, and interface engineering will lead to further improvement of perovskite solar cell devices.

*Un-certified results. Certification is underway.

Structure Prediction of Zinc-Oxide Surfaces

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To understand the properties of zinc-oxide (ZnO) surfaces, it is of paramount importance to first understand their atomistic structure. Not only do microscopic structural details directly impact the interfacial electronic structure in hybrid inorganic/organic devices, but they must also be expected to indirectly affect (opto) electronic properties through dictating the growth mode of an organic semiconductor deposited onto ZnO. Also a targeted tailoring of the inorganic/organic interface towards application-specific demands, e.g., through introducing self-assembled monolayers (SAMs) of covalently bonded molecules, hinges on a precise knowledge of the resulting surface structure. Here, I will give an overview over ongoing work in project A4, covering progress in (i) structure and stability prediction of bare and SAM-covered ZnO surfaces, (ii) correlating predicted structures with experimentally accessible quantities such as core-level shifts, and (iii) reaction paths and barriers encountered upon functionalizing of ZnO surfaces with SAMs. Time permitting, I will then briefly summarize the status of joint efforts with other projects in CRC 951.