Analysis of Electronic Structure and Surface Local Structure of Metal Oxides Thin Film for High Efficiency Organic Photoelectric Device

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Keywords: NEXAFS, UPS, charge extraction, charge iinjection, electronic structure, metal oxide

During the last few years, metal oxides (MO) such as titanium dioxide (TiO2) and zinc oxide (ZnO), have been extensively studied because of their exceptional optical and electronic properties for not only gas sensors and catalysts but also optical devices as charge injection and extraction layers in organic light emitting diodes (OLED) and organic photovoltaic (OPV) cells. Spin-coating method by using nanoparticles provides high quality MO layers due to their small particle size, The surface structure of nanoparticles such as vacancies and surface hydroxy groups largely affects the valence electronic properties, The efficiency of the devices, which include MO nanoparticles layer, depend on the interface electronic structure between MO nanoparticle layer and charge transport layer such as organic semiconductor layer in OLED and OPV cells. We analyze the valence electronic structure of annealed TiO2 nanoparticles, and nitrogen (N) doped ZnO nanoparticles by means of near-edge X-ray absorption spectroscopy (NEXAFS), ultraviolet photoelectron spectroscopy (UPS) and x-ray photoelectron spectroscopy (XPS). The annealing conditions such as temperature and atmosphere affect the introduction of oxygen vacancies into the surface of TiO2 nanoparticles. These annealing conditions make the impact of the valence band structure. For the case of N doped ZnO, the doping concentrations are determined by XPS. The NEXAFS provide the information on the local structure of around N atom such as the existing of N - Zn bond in N doped ZnO. Furthermore, the valence band top shifts to the Fermi level by N doping, which indicates the possibility of providing the p-type characteristic to N doped ZnO.

Application of spontaneous orientation polarization to electret-based vibrationale energy harvesters

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Keywords: electret, energy harvesting, organic light-mitting diodes, orientation polarization, surface potential

Electret-based vibrational energy harvesters (E-VEHs) have garnered significant attention due to their ability to provide relatively high output power even at frequencies in the range of several tens of Hz. Furthermore, they can be miniaturized using microelectromechanical systems (MEMS) technology. However, practical realization of E-VEHs remains limited due to the complex fabrication process, primarily the charging process for dielectric materials.

To circumvent the need for a charging process during electret preparation, our group proposed the use of polar organic molecules, such as Alq3 and TPBi, originally developed for organic light-emitting diodes (OLEDs) as electrets. The surface potential of the film composed of these molecules is built up without any charging process, thanks to the spontaneous orientation polarization (SOP) [1,2]. By leveraging these molecules, we developed E-VEHs without the need for any charging process, suggesting that polar organic molecules can be considered as "self-assembled electret" (SAE) [3,4].

We believe that the application of SAE to E-VEHs opens up new possibilities for device development. In this talk, we will introduce the operational mechanism of SAE-based VEHs and discuss the impact of light irradiation on the device lifetime [5,6].

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Buried interface regulation of perovskite thin films and high-efficiency fully-printed carbon-based perovskite solar cells

by Dongjie Wang | Guilin University of Electronic Technology

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Keywords: Buried interface, Carbon electrode, Fully-printed, Mesoscopic, Perovskite thin films

Carbon-based mesoscopic perovskite solar cells (C-MPSCs) fabricated by fully-printed technology have advantages such as high stability, low cost, and ease of large-scale preparation. Due to the unbalanced carrier transport and extraction at the buried interface between perovskite thin film and mesoporous electron transport layer, the power conversion efficiency of C-MPSCs is lower than that of traditional PSCs. To address the key scientific issue of energy loss at the buried interface, our team introduced guanidine sulfate (GUA_2SO_4), which has a synergistic effect of anions and cations, into C-MPSCs as an interface regulation material. SO_4^{2-} preferentially interacts with Pb^{2+} in the perovskite film to form water-insoluble lead sulfate compounds, which effectively reduces the formation sites of Pb-related defects in the perovskite film; GUA^+ diffuses to the grain boundaries of perovskite film, inducing the formation of low-dimensional perovskite, and effectively suppressing the energy loss caused by non-radiative recombination at the grain boundaries of the film. Besides, the introduction of GUA_2SO_4 can optimize the energy level arrangement at the buried interface of perovskite films, while reducing the oxygen vacancy concentration on the surface of TiO_2 films and enhancing electron extraction at the buried interface. In conclusion, this report shares an effective method for preparing high-efficiency C-MPSCs by buried interface control of perovskite thin films.

Carbon Electrode Interface Modulation in Fully Printable Mesoscopic Perovskite Solar Cells

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Keywords: carbon-based perovskite solar cells, fully printable, interface modulation, power conversion efficiency, voltage losses

Organic-inorganic hybrid perovskite solar cells have attracted significant attention due to their excellent power conversion efficiency (PCE), cost-effectiveness, and straightforward fabrication processes, showing promising prospects for application. Before industrializing PSCs, the challenges of producing large-area modules and obtaining long-term stability must be addressed. The fully printable hole-conductor-free mesoscopic perovskite solar cells (p-MPSCs) based on a prefabricated triple mesoscopic layer exhibit advantages in this aspect. However, further improvement in the efficiency of p-MPSCs is hindered by the low hole extraction efficiency at the perovskite/carbon electrode interface. Herein, we employed 1-naphthylmethylamine (NMA) post-treatment on p-MPSCs. The aromatic conjugated framework of NMA with π-electron delocalization enhances charge transfer at the interface of perovskite and carbon electrodes. Furthermore, the amine groups of NMA selectively react with surface methylammonium ions and lead iodide, resulting in the generation of low-dimensional perovskite and the formation of a type II energy level alignment at the interface of the perovskite and carbon electrode. Consequently, NMA suppressed the recombination assisted by defects in p-MPSCs, adjusted the energy band alignment at the interface of perovskite and carbon electrode, and increased the open-circuit voltage (V_{OC}) of p-MPSCs to 1050 mV. As a result, the power conversion efficiency (PCE) of p-MPSCs increased from 17.51% to 19.60%. This post-treatment strategy, utilizing the unique structure of the three-layer mesoporous architecture, offers novel insights into the inhibition of non-radiative recombination, reduction of V_{OC} losses in the devices, and improvement of their performance.

Charge separation enabled by intramoiety delocalized excitations in organic photovoltaic materials

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: charge separation, organic photovoltaic, ultrafast spectroscopy

Organic photovoltaic (OPV) devices that utilize non-fullerene acceptors have shown better compatibility in device configurations with larger active layer domains. In these setups, charge separation is efficient even with minimal energy loss at the interfaces. However, the exact process behind this improvement has been unclear. Through the use of broadband ultrafast spectroscopy, we've discovered a crucial step involving the delocalization of excitation within a single molecular entity that facilitates charge separation. This process bypasses the need for tightly bound charge-transfer states at the interface, addressing the issue of limited exciton diffusion distances common in organic materials. The discovery of this long-distance charge separation method, alongside the known short-distance interface-based mechanism, opens new avenues for enhancing OPV efficiency across various device architectures.

Charge Transfer Doping and Atomic Layer Deposition toward WSe2-FET via Self-Assembled Monolayer using F6-TCNNQ

by Kensho Matsuda | Daisuke Horiba | Takuya Kojima | Kohei Sakanashi | Mengnan Ke | Shohei Kumagai | Toshihiro Okamoto | Nobuyuki Aoki | Chiba University | Chiba University | Chiba University | Chiba University | Chiba University | Tokyo Institute of Technology | Tokyo Institute of Technology | Chiba University

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Keywords: ALD, Doping, F6-TCNNQ, SAM, TMDC

Doping effect is one the most important issues in the practical use of 2-dimensional (2D) materials such as transition metal dichalcogenide (TMDC) for the channel materials of 2D-field effect transistor (FET) in the future logic circuits. In this study, we demonstrate p-type doping for a few-layers crystal of WSe_2 via charge transfer doping using a self-assembled monolayer (SAM). Hexafluoro-tetracyano-naphthoquinodimethane (F6-TCNNQ) is one of the promising molecules for acceptor due to the electron affinity level deeper than the valence band edge of a monolayer WSe_2. In addition, it has a flat-molecular structure and a highly electron attracting characteristics by halogen atoms. Due to the strong van der Waals instruction via flat structure, a selective growth of a self-assembled monolayer (SAM) can be expected on the surface of the 2D materials. Such a SAM layer could be useful as a seed layer for atomic layer deposition (ALD) of high-*k* metal oxide in 2D-FETs composed of TMDCs in the future VLSI [1]. Using a vacuum-tube furnace, selective growth of the SAM layer of F6-TCNNQ has been achieved on a WSe_2-FET at appropriate temperature without deposited on the other region such as metal electrodes and SiO_2 on the substrate. After the depositions, clear positive shift of the threshold voltage without degradation of the mobility and the on/off ratio as shown in Fig. 1. Moreover, we confirmed that the contact resistance between the metal (Pd or Pt) and the WSe_2 have also been improved more than one order of magnitude after the deposition of F6-TCNNQ on the top of the FET channel as the second-order effect. Using the SAM layer, we are trying to deposit high-*k* metal oxide on the WSe_2. This work is supported by Tokyo Electron Limited.

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Conduction band structure of organic semiconductors and partially-dressed polaron formation

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Keywords: conduction band, energy band structure, low-energy inverse photoelectron spectroscopy, mobility, polaron

The energy band structure (the energy-momentum dispersion relation) provides crucial information on charge transport in organic semiconductors, such as transfer integrals and electron-phonon coupling. Whereas the experimental observation of the valence band (HOMO) structure has been reported since the 1990s, the conduction band (LUMO) has yet to be experimentally observed.

Recently, we have developed angle-resolved low-energy inverse photoelectron spectroscopy (ARLEIPS) [1]. We apply ARLEIPS to pentacene, a prototypical high-mobility organic semiconductor, to successfully observe the conduction band structure of organic semiconductors for the first time [2]. To address the observed bandwidths, we propose an improved polaron model, called partially-dressed polaron moel, that accounts for the electron-intramolecular vibrational interaction with frequency-dependent coupling constants. The new model successfully explains the inferior mobility of the electron (the n-type semiconductor property) to that of the hole (the n-type semiconductor property).

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Conjugated polyelectrolytes are compatible with perovskites : Their diverse applications in perovskite optoelectronic devices

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: conjugated polyelectrolyte, perovskite devices

The exceptional magnetic, electrical, and optical properties exhibited by metal halide perovskites (MHPs) have garnered significant interest from the optoelectronic research community in recent decades. These materials have found wide-ranging applications in photovoltaics, light emitting diodes, lasers, photodetectors, field effect transistors, and solar concentrators.

To optimize the performance and stability of perovskite light emitting diodes (PeLEDs) and solar cells (PeSCs), it is crucial to incorporate appropriate charge transport layers (CTLs) and/or interlayers. These CTLs need to possess suitable energy levels for efficient charge injection and transport, while effectively blocking opposite charges. Additionally, the CTL located beneath the perovskite layer plays a critical role as it significantly influences the crystal growth of the perovskite layer and affects the presence of interfacial defects. In this presentation, a new series of conjugated polyelectrolytes (CPEs) will be introduced as ideal interfacial layers and CTLs for various PeLEDs and PeSCs devices.

Density of states of in-gap states of organic semiconductors determined by photoemission total and partial yield spectroscopies using low-energy photons: Observation of the initial density of states, exciton fusions, and negative-polarons

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Constant final state yield spectroscopy, Organic semiconductor, Photoemission yield spectroscopy, in-gap states

Weak electronic states between HOMO and LUMO, so-called in-gap states, effects organic optoelectronic devices. Determining the density of states (DOS) of in-gap states is essential to understanding carrier traps and vacuum level shifts at organic/metal interfaces. Photoemission yield spectroscopy (PYS), which measures the photoemission total yield with changing low-energy photons, has been utilized to investigate the ionization energy of semiconductors by device field researchers. Recently, Nakano *et al.* suggested that the differential spectrum of PYS reflects the DOS of in-gap states [1]. However, when using low-energy photons such as those used in PYS, photoemission that cannot be attributed to the initial DOS has been reported. In the inorganic semiconductors field, constant final state yield spectroscopy (CFS-YS), which is photoemission "partial" yield spectroscopy at specific kinetic energy, has been used for measuring the DOS of in-gap states.

In this study, we applied PYS and CFS-YS to organic semiconductors to establish a way to determine the DOS of in-gap states. In low-energy photon irradiation, we observed photoemissions assigned not only as the initial DOS but also as negative-polaron and exciton-exciton fusion caused auto-ionization (EEF-AI). In that case, the differential spectrum of PYS had artificial peaks due to EEF-AI, indicating that the differential spectrum of PYS cannot determine the DOS of in-gap states. This is because PYS cannot distinguish the initial DOS, negative-polaron, and EEF-AI from photoelectrons. We revealed that CFS-YS can determine the correct DOS by performing CFS-YS at kinetic energy where EEF-AI is undetected. In the case of Alq3, CFS-YS can determine the DOS of HOMO, in-gap states, and negative polarons. Furthermore, we show the criteria for when PYS can be used. In our presentation, we will also discuss the detailed results of EEF-AI.

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Design Strategy of Organic Semiconducting Materials for Organic Electronics

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Keywords: OLED, OPV, OTFT, organic electronics

Over the past two decades, organic electronics, such as organic field-effect transistors, organic light

emitting diodes, organic photovoltaic cells, and organic photodetectors have recently received significant attention for use in flexible low-cost electronics applications.

The molecular design of organic semiconductors is a useful strategy for high performance organic solar cells, organic thin film transistor because tailoring the molecular structures can dramatically tune the properties of the organic semiconductors. In this presentation, I will introduce the design strategy of organic semiconducting materials for various organic electronics applications.

Development of new film processing by sol-gel method and electronic structure of nitrogen doped ZnO

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Annealing, Bonding state, Doping, Photoelectron spectroscopy, Zinc oxide

Zinc oxide (ZnO) is considered a very promising material for optoelectronic devices. Unfortunately, the advantage of such a newly technology suffers of the lack of easily obtainable p-n homojunctions. Until now, the fabrication of reliable p-type ZnO thin film has been a bottleneck, Nitrogen, having an ionic radius comparable to oxygen, appears to be the most likely dopant candidate.

In this study, we aim to develop a new fabrication process that achieves highly efficient N doping into ZnO (NZO) thin films by clarifying the changes in structure and chemical state around the dopant nitrogen (N) atoms. We obtain the information on the N doping such as dopant concentration and the bonding state for N atoms in NZO by x-ray photoelectron spectroscopy (XPS) and x-ray absorption near edge fine structure (NEXAFS). Furthermore, we estimate the effect of doping on the valence band structure by using ultraviolet photoelectron spectroscopy (UPS). The annealing temperature affects largely the bonding state around the N atom. The heating process at 450℃ provides the p-type doping by replacing an oxygen atom by a nitrogen atom. At temperatures higher than 450℃ the concentration of N atom in NZO decreases. There is a possibility that at temperatures higher than 450℃ the N-N bonds form and N_2 molecules eliminate from NZO thin films. The results of UPS show that the position of the valence band maximum (VBM) shifts toward the Fermi level, which exhibits p- type characteristics. These results indicate that the bonding state of dopants and the valence electronic structure such as VBM can be controlled by fabrication conditions of N doped ZnO thin films.

Direct imaging of the inherent functionality of molecular machines on host crown ether array

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Keywords: crown ether, ferrocene, host-guest complex, molecular machine, scanning tunneling microscopy

Artificial molecular machines, specifically motors based on wheel-and-axle complexes, hold immense promise for mechanical motions in response to external stimuli. These minute motions have yielded substantial advancements in robotic molecular apparatus. Using ammonium-ion tethered ferrocene (Fc) as the mobile “guest” axle, we conducted on-surface molecular machine fabrication via the utilization of a two-dimensional crown ether (CR) self-assembled monolayer (SAM) nanoporous film [1,2] as the “host,” constructed atop an atomically flat Cu(111) surface.

Herein, we present a novel bottom-up methodology to elucidate the structure-property correlation on the surface employing an ultrahigh vacuum (UHV) cryogenic scanning tunneling microscopy and spectroscopy (STM/STS) setup, complemented by X-ray photoelectron spectroscopy and density functional theory calculations.

We found that the capability to capture the guest Fc compounds at 300 K in an ultrahigh vacuum without undergoing decomposition suggests that the CR film serves as an electronic decoupling layer from the substrate. Despite the guest being trapped by the host nanopores in the connection, the guest is liberated from the trap in the array, exhibiting internal motion when the hole is injected into the Fc orbital, thereby initiating Fc ring rotation. This revelation exposes an advanced pathway for constructing the Fc-based single-molecular nanomachine junction utilizing a Cu metal surface through the on-surface bottom-up process under vacuum conditions at ambient temperature.

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Effects of energy level alignment on the operating voltage of organic light-emitting diodes

by Taku Oono | Tsubasa Sasaki | Takuya Okada | Takahisa Shimizu | NHK | NHK | NHK | NHK

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Organic light-emitting diode, electron injection, energy level alignment, hole injection, low work function

Organic light-emitting diodes (OLEDs) have been intensively studied as a promising technology for mobile displays, televisions and solid-state lighting. The efficiency of light-emitting materials has been improved significantly through the discovery of both phosphorescent and thermally activated delayed fluorescent emitters. However, the correlation between the energy level alignment and the operating voltage in OLEDs remains unclear, because OLEDs require a complex multilayer configuration that includes many materials other than the emitter. It is difficult to investigate the exact energy diagram for OLEDs, which have many interfaces, and many uncertainties remain regarding the mechanisms of charge injection. In this talk, we introduce both the charge injection mechanisms in OLEDs and the interface control technology effective for lowering the operating voltage of OLEDs. We have obtained a complete understanding of the electron injection mechanism at organic/cathode interfaces by using organic bases as the electron injection layers [1, 2, 3]. The hole injection mechanism in OLEDs was also clarified by investigating the correlation between characteristics of OLEDs with the actual energy levels at organic/anode interfaces [4]. With the elucidation of the charge injection mechanism, holes and electrons can be injected into a variety of organic materials [4, 5]. These charge injection techniques minimize the voltage required for charge recombination, and by tuning the energy levels at the organic/organic interface, blue and green OLEDs that emit light at voltages at about 1.5 V are realized [6].

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Effects of partially dressed polaron formation on mobility of organic semiconductors

by Hiroyuki Ishii | Hiroyuki Yoshida | Nobuhiko Kobayashi | University of Tsukuba | Chiba University | University of Tsukuba

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Charge transport, Organic semiconductors, dynamic disorder, polaron, simulation

Charge mobility is an important factor that dominates performance such as cutoff frequency of field-effect transistors and photoelectric conversion efficiency of solar cells. The electron mobilities observed in experiments using single crystals are often lower than the hole mobilities. Namely, n-type organic semiconductors with low mobility limit the performance of organic devices consisting of p and n-type semiconductors. However, the microscopic origin of low electron mobility remains an open question.

In organic semiconductors, charge is strongly coupled with molecular vibrations. Unlike inorganic semiconductors, transfer integrals t (electronic bandwidth) of organic semiconductors are small and comparable to the molecular vibration energy $\hbar w$. Previous theories often assume that the high-frequency intramolecular vibrations ($\hbar w > t$) form a “polaron” in which a charge is dressed in the molecular distortion clouds while the slow intermolecular vibrations ($\hbar w < t$) induce “dynamic disorder” in transfer integrals. However, we found these may be insufficient to explain the difference in mobility between electrons and holes.

Recently, we proposed a *partially dressed polaron* picture, which can quantitatively explain the valence and conduction band modulation observed by state-of-the-art photoelectron and inverse photoelectron spectroscopies [1]. In this presentation, we propose our time-dependent wave-packet diffusion (TD-WPD) method [2], which enables us to calculate the charge mobilities taking both dynamic disorder and partially dressed polaron. We applied the method to several p and n-type organic semiconductors. Our calculated results suggest that the low-frequency intramolecular vibrations largely reduce the electron mobility in comparison with hole mobility. We will discuss the detail in our presentation.

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Efficient and stable perovskite optoelectronic devices via charge carrier transport modulation and defects passivation

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Perovskite solar cells, charge carrier transport modulation, defects passivation, perovskite light-emitting diodes

Halide perovskite materials own excellent semiconductor properties, which shows great potential in photovoltaic, emission display . In this talk, firstly, I will talk about the halide perovskite materials and its application in optoelectronic devices, and then focus on talking about our group’s progresses in high performance perovskite solar cells and perovskite light-emitting diodes via charge carrier transport modulation and defects passivation. 1) Halide salts passivation for over than 26% efficiency perovskite solar cells, 2) Perovskite thin film growth crystal and module design leading to 23% perovskite mini-module; 3) Deep level molecular doping leading to very efficient blue emission perovskite light-emitting diodes.

Efficient blue delayed fluorescence molecules with ultrafast bipolar charge transport for simplified non-doped thick-layer organic light-emitting diodes

by Zujin Zhao | South China University of Technology

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Keywords: organic light-emitting diode; thermally activated delayed fluorescence; aggregation-enhanced emission; hyperfluorescence; bipolar charge transport

Organic molecules with strong photoluminescence and fast charge transport simultaneously are highly desired in optoelectronic devices but remain challenging because of the trade-off between these properties. Herein, two blue molecules constructed with ring-fused carbonyl-containing electron acceptors with delocalized π-electrons and spiro-acridine electron donors are developed. Owing to ordered long-range alignment with proper interaction energies of the molecules, their neat films have strong delayed fluorescence with high photoluminescence quantum yields and short delayed fluorescence lifetimes, and ultrafast bipolar charge transport. In doped organic light-emitting diodes (OLEDs), both molecules display eminent electroluminescence performances with excellent external quantum efficiencies (EQEs) of 40.6%. They also exhibit brilliant blue lights with record-beating EQEs of 30.2% in non-doped thin-layer OLEDs, and more importantly, high-performance simplified non-doped thick-layer OLEDs are achieved, rendering lowered driving voltages, improved operational stability and the best EQEs of 23.0% with tiny efficiency roll-offs. The ultrafast bipolar charge transfer capability enables efficient exciton recombination in a broadened zone, and the thick emitting layer is more beneficial for lowering exciton density and alleviating exciton quenching. This work provides promising candidates for highly efficient simplified thick-layer OLEDs and opens a new avenue for exploring organic molecules with strong photoluminescence and fast charge transport simultaneously.

Energy-Efficient Stable Hyperfluorescence Organic Light-Emitting Diodes with Improved Color Purities and Ultrahigh Power Efficiencies Based on Low-Polar Sensitizing Systems

by Hao Liu, Yan Fu, Jinke Chen, Ben Zhong Tang, Zujin Zhao | South China University of Technology

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: hyperfluorescence, low-polar sensitizing systems, multi-resonance, organic light-emitting diodes, thermally activated delayed fluorescence

Multi-resonance (MR) molecules with thermally activated delayed fluorescence (TADF) are emerging as promising candidates for high-definition displays because of their narrow emission spectra. However, the electroluminescence (EL) efficiencies and spectra of MR-TADF molecules are highly sensitive to hosts and sensitizers when applied to organic light-emitting diodes (OLEDs), and the highly polar environments in devices often lead to significantly broadened EL spectra. In this study, a proof-of-concept TADF sensitizer (BTDMAC-XT) with low polarity, high steric hindrance, and concentration-quenching free feature is constructed, which acts as a good emitter in doped and non-doped OLEDs with high external quantum efficiencies (ηexts) of 26.7% and 29.3%, respectively. By combining BTDMAC-XT with conventional low-polarity hosts, low-polarity sensitizing systems with a small carrier injection barrier and full exciton utilization are constructed for the MR-TADF molecule BN2. Hyperfluorescence (HF) OLEDs employing the low-polar sensitizing systems successfully improve the color quality of BN2 and afford an excellent ηext of 34.4%, a record-high power efficiency of 166.3 lm W−1 and a long operational lifetime (LT50 = 40309 h) at an initial luminance of 100 cd m−2. These results provide instructive guidance for the sensitizer design and device optimization for energy-efficient and stable HF-OLEDs with high-quality light.

Enhanced light absorption and stability of perovskite solar cells through grating-structured PEAI/2D perovskite interfacial layer

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Keywords: 2D perovskite, interface engineering, nano-imprint, perovskite solar cells

Interface engineering passivation and micro-nanostructure management of light are very effective methods to improve the performance of perovskite solar cells (PSC) nowadays. Here, we used thermal imprinting to transfer a PEAI layer on the perovskite layer. PEAI can react with excess PbI_2 on the surface of perovskite to form 2D perovskite, resulting in a PEAI/2D perovskite interface layer with a grating structure. The grating structure effectively scatters incident light, increasing the light absorption of the PSC, while the interface layer effectively passivates the perovskite's surface defects. Compared with the control device, the power conversion efficiency of the device with the interface layer increased from 19.87% to 22.45%. At the same time, the device with the interface layer has excellent thermal stability due to the reduction of surface defects. It can retain 90% initial effectiveness after 550 hours in an 85℃, N_2 atmosphere. This method of coupling interface engineering passivation and micro-nano structure offers a novel strategy for enhancing the stability and performance of PSCs.

Enhanced Terahertz Generation in Nonlinear Thin film Crystals

by Dongwei ZHAI | Qingdao university

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Keywords: organic/inorganic crystal, terahertz photonics, thin film crystal

Optical rectification (OR) is a well-known and elegant way to generate intense and broadband terahertz (THz) pulses in nonlinear crystals [1]. The optical/THz conversion efficiency is mainly governed by the phase-matching condition, the crystal nonlinearity, and losses at optical and THz frequencies [2]. Semiconductors are known to exhibit an enhanced nonlinear susceptibility in the vicinity of their bandgap [3], especially when dealing with second harmonic generation, Kerr, and electrooptic effects. The propagation of the optical beam with high photon energy becomes very weak in the crystals. It is possible to reduce the optical loss by using thin film crystals. Thus, we propose to take the benefit of the same bandgap enhancement to produce intense THz pulses in thin film crystals.

In this work, we perform THz generation in GaSe (ZnTe, KTP, and DAST) bulk and thin film crystals with femtosecond laser pulses under normal incidence, whose photon energy ranges below and above the crystal bandgap [4-6]. We observe a strong THz emission when the pump photon energy reaches the crystal bandgap, and an increased optical loss when the crystal thickness is over its maximum phase-matching distance. Additionally, for the first time, we report an enhanced broadband THz emission in a 20-um GaSe crystal, which could bring new possibilities for thin film THz sources. The results are analyzed using a nonlinear dielectric model. This phenomenon is explained by the resonance theory of material nonlinear susceptibility around its bandgap.

Enhancing Indoor Perovskite Photovoltaics through the Implementation of Bilayer Hole Transport Layers

by Chih-Ping Chen | Ming Chi University of Technology

Abstract ID: 10036
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: perovskite solar cell; indoor harvesting; self-assembly layer

The burgeoning interest in self-powered integrated IoT devices, capable of harvesting energy from indoor photovoltaics, has spotlighted Perovskite solar cells (PSCs). These cells have attracted considerable attention owing to their efficient performance and favorable solution process, establishing them as a preferred solution for mitigating the energy consumption challenges associated with the Internet of Things.[1] Successfully enhancing the efficiency of PSCs involves the effective mitigation of interfacial defects through the incorporation of a hole transporting layer (HTL).[1] This study utilized a bilayer HTL structure incorporating sol-gel nickel oxide (NiO_x) and self-assembled (SA) layers for PSCs. The application of (2-(9H-carbazol-9-yl)ethyl)phosphonic acid (2PACz) and its derivatives effectively addressed defects in both NiO_x and perovskite interfacial regions, promoting energy alignment at the HSL/perovskite interface and enhancing carrier transport efficiency. Under 3000K LED illumination at 1000 lux, the indoor light performance showcased an optimized efficiency exceeding 41% for $Cs_{0.18}FA_{0.82}Pb(I_{0.8}Br_{0.2})_3$. Comprehensive characterization studies, including atomic-force microscopy images, X-ray diffraction patterns, X-ray photoelectron spectroscopy, photoluminescence (PL) spectra, and time-resolved PL curves, supported the successful passivation of defects in the devices. These findings underscore the potential of bilayer HTL-based interface modification as a practical and promising approach for improving passivation and contact properties, ultimately contributing to the development of high-performance PSCs.

(1) Enhancing the Efficiency of Indoor Perovskite Solar Cells through Surface Defect Passivation with Coplanar Heteroacene Cored A–D–A-type Molecules. *Advanced Functional Materials* , 2312819. DOI: https://doi.org/10.1002/adfm.202312819.

Epitaxy and doping of metal halide perovskite semiconductor thin films

by Bingqiang CAO | Lifang Xu | University of Jinan | University of Jinan

Abstract ID: 10470
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Epitaxy, doping, perovskite semiconductor, thin films

Modern semiconductor devices require materials with a variety of lattice constants, thermal expansion coefficients, electrical conductivity and crystal orientations. Therefore, epitaxy technology has attained great attention for several decades and it is expected to grow almost any semiconductor material with unprecedented control on composition uniformity and electrical conductivity. As an typical epitaxial technology, pulsed laser deposition (PLD) can provide a potential approach for manufacturing high-quality and sophisticated inorganic compound films with the aim of transferring their applications from the laboratory to the market.

Recently, the application of metal halide perovskite semiconductor materials in high-performance solar cells, X-ray detection, and other thin film electronics has been a research hotspot. In this talk, we will present the progress of inorganic halide perovskite thin films that were epitaxially grown on different substrates by PLD including their primary application in photodetectors and solar cells.

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Exploring Photoexcitation Dynamics in Perovskites Using Ultrafast Broadband Photoluminescence Spectroscopy

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Abstract ID: 10512
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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Ultrafast spectroscopy, optoelectronic materials, perovskite, photoexcitation dynamics, photophysics

Perovskite-based semiconductors have emerged as a central subject of study in optoelectronics due to their remarkable potential across a variety of applications.[1] The performance and optoelectronic characteristics of these materials are profoundly influenced by their photoexcited states. A deep understanding of photoexcitation dynamics, including exciton behavior and carrier-phonon interactions, is crucial for both advancing our knowledge of perovskite materials and enhancing their practical performance. Here, we will highlight recent research that illuminates the photoexcitation dynamics within perovskites. Employing our patented technique of transient grating photoluminescence (PL) spectroscopy,[2] we investigate these interactions at ultrafast timescales, capturing transient PL spectra from sub-picoseconds to picoseconds. This method represents a significant advancement over traditional transient absorption techniques, offering a more intuitive interpretation of data. By providing insights directly related to perovskites' key optoelectronic feature—photoluminescence—our approach promotes a more immediate understanding of key material properties. This approach enables a clearer comprehension of essential characteristics crucial for semiconductor laser and laser cooling technologies,[3.4] thereby providing valuable insights into enhancing perovskite materials for their use in optoelectronic applications.

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Extracting Charge Carrier Mobility in Organic Solar Cells

by Hang Yin | Shandong University

Abstract ID: 10045
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Charge carrier transport; Space-charge-limited current measurement

Mobility is a critical parameter influencing the overall performance of organic solar cells (OSCs). Herein, we innovatively elucidated the intricate interrelation between the photovoltaic molecular structures and the methodologies employed for the extraction of charge carrier mobility in OSCs. We proposed a simple yet effective principle to accurately extract charge carrier mobility values using the standard space-charge-limited current (SCLC) measurement, while critically assessing theoretical and experimental deficiencies through the drift-diffusion analysis. It was found that field-dependent charge transport is necessitated to describe the prominent long-range intrachain hopping carrier behavior in polymers, while short-range intermolecular hopping results in trap-involved charge transport within small molecular acceptors. Based on the above understanding, a synergetic inter/intra-molecular hopping strategy was proposed to fabricate thick-film all-polymer OSCs, and an unprecedented power conversion efficiency (PCE) of 16.61% was achieved in the 300 nm PM6:PY-IT OSC. This work not only presents a precise and straightforward approach for measuring mobility values, but also provides a significant reference about charge carrier transport to make optimal decisions regarding photovoltaic material design and device fabrication process of high-performance OSCs

Film structure and electronic structure of poly(3-hexyl)thiophene (P3HT) doped with 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ)

by Yugo Hoshi | Koji Okudaira | Chiba Univ. | Chiba Univ.

Abstract ID: 10399
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: film structure, organic semiconductor devices, photo electron spectroscopy, polymer

Recent research focuses on improving organic semiconductor devices' efficiency by doping electron-donating or accepting substances into organic layers. P3HT, a typical polymer-based semiconductor, shows high conductivity by F4TCNQ doping. Two solution processes for doping have been reported, one is sequentially solution deposition method the other is the standard mixed-solution method, with the former demonstrating high conductivity. The aim of this study is to compare the electronic structure and properties of films by sequentially doping with those by the standard mixed-solution method for achieving P3HT organic layer with high conductivity.

We estimate the doping amounts by quantitative analysis using XPS. It is found that for the case of sequential film deposition, there is a high possibility of surface segregation of the dopant. In the UPS, the changes of the valence band structure due to doping are observed for both the mixed method and sequential deposition method samples, with the HOMO onset approaching the Fermi level. Particularly in the samples prepared by sequential deposition, the HOMO onset shifts to near the Fermi level, suggesting the potential for higher conductivity. NEXAFS measurements reveal that the films prepared by the sequential method exhibits the same edge-on orientation as undoped highly crystalline P3HT, indicating no disruption in molecular orientation due to doping. On the other hand, the samples prepared by the mixed method shows a reduction of average tilt angle of P3HT molecules, suggesting a possibility of decrease in the crystallinity of P3HT due to the presence of the dopant. The cause of the high conductivity observed in films prepared by sequential deposition is found to involve minimal disruption in the film structure due to doping, and changes in the electronic structure near the Fermi level.

Fluorescence lifetime dynamics: Investigating Alq3 Luminescence with Cu, In, Ga and Sn Metal Layers in Alq3/metal/Alq3 Thinfilm Multi-Stacks

by P Issac Nelson | A Mohan | Jayaramakrishnan Velusamy | Sam Zhang | ANEH Scientific Foundation, Karur, Tamil Nadu, India | Department of Physics, St. Joseph's University, Bengaluru-560027, India | Department of Chemical Engineering and Biotechnology, University of Cambridge, Philippa Fawcett Drive, Cambridge, CB3 0AS, United Kingdom | School of Aeronautics, Harbin Institute of Technology, Harbin 150001 China & Zhengzhou Research Institute, Harbin Institute of Technology, Zhengzhou, 450000 China

Abstract ID: 10360
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Alq3, Emission, Fluorescence lifetime, Metals., Multistacks, Thinfilm

Tris-(8-hydroxyquinoline) aluminium (Alq_3) is a well-established material in the electron transport and emission layers of organic light-emitting diodes (OLEDs). However, the pursuit of more efficient and versatile emissive systems has led researchers to explore the potential of metal-organic frameworks and metal-organic-metal structures in this domain. In particular, the interface between the metal electrode and the organic layer has emerged as a promising area for enhancing the fluorescence dynamics and metal-organic interactions of thinfilm emissive layers. Despite these efforts, much remains to be understood about the optimal design of metal-organic emissive thinfilm layers. To address this, we experimented to investigate the luminescence of Alq_3 in the context of metal incorporation in thin film Alq_3/metal/Alq_3 multi-stacks. We selected Copper (Cu), Indium (In), Gallium (Ga), and Tin (Sn) as the variable metals and used X-ray diffraction analysis to confirm their presence in the multistacks. The organic Alq_3 layer showed no changes in meridional isomerism despite variations in metal-bond vibrations. However, there were significant differences in the morphological features of the multistacks depending on the metal used. The growth epitaxy and polymeric fibres were retained only in Ga and In added metal-organic systems. Ultraviolet absorption spectroscopy showed ligand-centered transitions with primary absorption in the UV region. Moreover, reflectance measurements and critical optical parameters such as refractive index and dielectric constants were scaled higher in stacks than in the monolayer. The conducted photoluminescent experiments to investigate the characteristic green emission of Alq_3 and the chromaticity CIE coordinates confirmed its unperturbed meridional isomerism. Fluorescence life decay profiles showed that 'In' metal-Alq_3 stacks exhibit the maximum lifetime amongst the films. Overall, our findings indicate that using metal-polymer stacks has opened exciting avenues for exploring alterations in the emissive and optical properties of Alq_3.

High Performance Organic Solar Cell Materials and Devices

by Qiang Peng | Sichuan University

Abstract ID: 10339
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: organic solar cells; donors and acceptors; blend morphology; device structure; efficiency

Bulk-heterojunction (BHJ) organic solar cells (OSCs), typically consisting of a polymer donor and a small molecular acceptor, have attracted extensive research attentions due to their unique features of low-cost large-area production, light weight, and mechanical flexibility. Recently, the PCEs of nonfullerene based OSCs have also increased beyond 19%. To further improve the performance of OSCs, the key materials including donor and acceptor materials along with the device structure and fabrication technology should be continuously researched.

In this presentation, we will report some advances in development of polymer donors and small molecular acceptors for efficient non-fullerene PSCs. The strategies include backbone design, side chain engineering, interface engineering. Also the new device structures and the new methods for optimizing the blend morphology will be presented. Based on these studies, PCEs more than 19% have been achieved in our group.

Highly Efficient Organic Solar Cells

by Ziyi Ge | Ningbo Institute of Materials Technology and Engineering, CAS

Abstract ID: 10338
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Organic solar cells, flexible, interfacial engineering, isomerization.

Organic solar cells have the advantages of low cost, light weight, flexibility and easy fabrication in large area. They have important application prospects in the fields of portable electronics, BIPV and military industry. We mainly introduce the progress in solution-processable flexible organic solar cells. Firstly, several solution processed non-conjugated small-molecule electrolytes were developed as cathode interfaces, leading to over 10% efficiency for single-junction OSCs. Secondly, flexible OSCs with acid-treated PEDOT:PSS electrode was prepared with the efficiency over 10%. By further using the natural green acid treated electrode, FST-OSCs was fabricated with over 10% efficiency and 21% average visible light transmittance, that could utilize visible light for plant growth and infrared light for power generation. We successfully designed and synthesized a novel small molecular donors G19 to construct ternary organic solar cells with outstanding PCEs of 18.5% for rigid and 15.9% for flexible OSCs, which are among the highest efficiency reported. Recently, we utilized interfacial engineering to achieve efficient organic solar cells with PCE 19.7% and flexible OSC with a record PCE over 18.2%.

High-performance all-polymer solar cells

by Yanming Sun | Beihang University

Abstract ID: 10285
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Organic solar cells, all-polymer blend, efficiency, morphology, stability

Polymer solar cells (PSCs) with merits of low cost, light weight, and flexibility have emerged as a promising next-generation clean energy. With the rapid development of small-molecule acceptors (SMAs), the power conversion efficiencies (PCEs) of SMA-based PSCs have undergone significant progress, demonstrating the great potential of the commercialization of PSCs. Actually, all-PSCs, which possess superior photo-thermal stability, mechanical robustness, and stretchability, are thought to be more suitable for the practical applications of PSCs. However, much less efforts have been devoted to all-PSCs, and the PCEs of all-PSCs lag far behind those of SMA-based PSCs. The main cause of the inferior performance of all-PSCs lies in the difficulty in morphology control. In this report, we will mainly talk about our recent progress on all-PSCs, including the molecular design of polymer acceptors, morphology control, thermal/photo-stability, energy loss and eco-friendly large-area device fabrication.

High-Performance Perovskite/Organic Tandem Solar Cells with Open Circuit Voltage Exceeding 2.2 V

by Jin Young Kim | Ulsan National Institute of Science and Technology (UNIST)

Abstract ID: 10580
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Mixed self-assembled monolayers, hole-selective layers, inverted perovskite solar cells, perovskite/organic tandem solar cells

Perovskite/organic tandem solar cells offer a promising avenue to surpass the Shockley-Queisser limit by mitigating thermalization losses. However, wide bandgap perovskite solar cells (WBG PSCs) face challenges, particularly in open-circuit voltage losses. Herein, we propose a novel approach employing a mixed self-assembled monolayer (mSAM) as a hole-selective layer (HSL). This strategy facilitates efficient hole extraction by homogenizing the surface potential of the HSL. Furthermore, the modification of indium tin oxide with mSAM enhances perovskite crystallinity, reducing lattice strain and phase segregation. Implementing mSAM on WBG PSCs enables a power conversion efficiency (PCE) of 18.85% with a notable VOC of 1.366 V and a high fill factor (FF) of 81.88%. When applied to fabricated POTSCs, the PCE reached 24.73% with a record-high VOC and FF of 2.216 V and 84.07%, respectively. These results demonstrate the potential of the mSAM strategy to advance both the performance and stability of perovskite-based tandem solar cells for practical renewable energy applications.

High-Performance See-Through Organic Solar Cells

by Chang-Zhi Li | Zhejiang University

Abstract ID: 10477
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Interfacial layer, Semitransparent, Solar cell, n-Doping

Thin-film solar cells made with polymer and perovskite absorbers represent a transformative technology with great potentials for high-throughput manufacturing at very low cost. In this talk, we will discuss the integrative approach of combining molecular design, interface and device to access high-performance polymer and perovskite solar cells, including the results of champion organic solar minimodules made in lab that have been published in the "Solar Cell Efficiency Table" by Prof. Martin Green (59th, 60th, 61st and 62nd editions), as well as our efforts in fabricating inverted perovskite solar cells with the certified efficiency over 26%.

Specific emphasis will be placed on the development of See-through power windows via a new design of semitransparent organic solar cells (ST-OSCs), which allows for the efficient utilization of spectrum-engineered solar photons from the visible to infrared range with both energy generation and saving features. Model analysis indicated that the installation of these see-through power windows worldwide would contribute to the carbon neutrality of society.

High-performance stretchable organic light-emitting devices based on wrinkles with controlled morphology

by Da Yin | Jing Feng | Jilin University | Jilin University

Abstract ID: 10484
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: OLEDs; stretchable; wrinkles

In recent years, stretchable light-emitting devices have attracted more and more attentions in recent years due to their potential applications in fields of deformable displays, electronic skin and biomedical devices. Among various electroluminescent (EL) devices based on different EL principles and materials, organic light-emitting devices (OLEDs) based on organic small-molecular materials have shown high efficiency and flexibility and been used in commercial displays, which promote the research of stretchable OLEDs. Wrinkled structures have been widely used for fabricating stretchable OLEDs with excellent optoelectrical and mechanical performance. For example, we have reported stretchable OLEDs based on regular wrinkles, which can achieve 100% elongation, current efficiency of 70 cd/A, and withstand 35,000 stretching-releasing cycles[1]. However, when facing practical applications, stretchable OLEDs based on wrinkled structures still face some problems, including light extraction loss caused by various optical modes in the devices, and display image distortion caused by the large size of the wrinkles.

To solve the above problems, we control and optimize the morphology of wrinkles to enhance the light extraction efficiency of the device by improving optical mode scattering[2] and reduce the size of regular wrinkles by reducing the thickness of the OLEDs substrate[3], so as to achieve stretchable OLEDs with high luminous efficiency and high display quality.

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High-Resolution Patterning of Fluorescent Films by Femtosecond Laser Direct Writing

by Yue-Feng Liu | Jing Feng | Jilin University | Jilin University

Abstract ID: 10504
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: High-resolution, femtosecond laser direct writing, fluorescent films, optoelectronic devices

High-resolution patterning techniques for fluorescent thin films are in extremely important demand in multiple application fields. Of particular concerns are displays, image sensor arrays, and fluorescent anti-counterfeiting labels. To date, several methods have been proposed to fabricate patterned fluorescent, such as photolithography, micro/nanoimprinting, and inkjet printing. However, the organic components in perovskite materials are sensitive to the chemical reagents in photolithography. Therefore, photolithography is not an ideal method for patterning perovskites. The micro/ nano-imprinting method suffers from the template deformation during the pressure process, which deteriorates the repeatability and fidelity. Inkjet printing is the most widely used patterning technique for organic and perovskite materials. However, it has a limitation in producing high-resolution patterning. A high-resolution of 5 μm has been successfully demonstrated using electrohydrodynamic printing. But the further improved resolution is difficult to realize because the nozzle capacity and a single injection volume of solution cannot be indefinitely reduced. Therefore, developing a suitable technique for high-resolution patterning of fluorescent film remains challenging.

Here, we proposed a facile femtosecond laser direct writing (FsLDW) to fabricate the patterned fluorescent film, involving the 2D (two-dimension), colloidal quantum dots and bulk perovskite. The femtosecond laser precision engineering has several advantages involving large-area, high-throughput, and far-field nanofabrication. The femtosecond laser allows a simple and reliable patterned ablation with a resolution of 200 nm, patterned deposition with a resolution of 1.58 μm and transferred deposition with a resolution of 1.78 μm. Due to the flexibility of the programmable femtosecond laser process, arbitrary patterns and arrays with different sizes of fluorescent films can be achieved. This facile-process, high-resolution and efficient patterning technique of fluorescent film provides a promising fabrication candidate for optoelectronic applications based on fluorescent materials.

Host Engineering for Efficient Cluster Light-Emitting Diodes

by Hui Xu | Heilongjiang University

Abstract ID: 10479
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Cluster, Emissive Layer, Exciton, Host, Light-Emitting Diode

Please note that the ThinFilms conference does not encourage multiple papers for one registration. Registration will be pegged to a paper ID: one paper per registration. A poster paper receives the same privilege as an oral paper. Of course, a corresponding author can be the same for multiple papers, but each paper should later have a different registered author participating the conference.

Electroluminescent (EL) clusters emerged rapidly in recent years, owing to their high photoluminescent (PL) quantum yields and organic-inorganic hybrid characteristics.[1] However, their complicated excited state composition and sensitivity to processing technologies still limit the material selection. Actually, before our works, there were no reports of EL CuI clusters based on monodentate ligands, because of the defects generated during film fabrication.

Our group has reported a series PL and EL Cu_4I_4 clusters with the high quantum efficiencies.[2] In our previous works, ligand engineering approaches were used to increase ligand-centered charge transfer states of the clusters, realizing top-rant quantum efficiencies up to 19.5%.[3] Most recently, we further develop host engineering strategy to externally optimize exciton ratios and allocation to radiative excited states of the clusters, further dramatically improving the quantum efficiencies to the up-limit of the planar devices as ~30%.[4] It is showed that host matrix can not only provide the additional triplet-to-singlet up-conversion channels through the reverse intersystem crossing of thermally activated delayed fluorescence (TADF) hosts,[5] but also passivate the defects at the interfaces and inside of cluster based emissive layers.[6] On the basis of these advantages, Cu_4I_4 clusters based on mono- and bi-dentate phosphine ligands achieved the state-of-the-art EL performances, making them promising for practical applications in display and lighting.

Impact of electron scattering on electronic states at the interface of chiral molecule-modified WS2 monolayer

by Fumi Nishino | Keisuke Fukutani | Jonas Brandhoff | Felix Otto | Marco Grünewald | Maximilian Schaal | Daniel Stelter | Julian Picker | Zheng Zhang | Andrey Turchanin | Takashi Hirose | Torsten Fritz | Satoshi Kera | Institute for molecular science | Institute for molecular science | Institute of Solid State Physics, Friedrich Schiller University Jena | Institute of Solid State Physics, Friedrich Schiller University Jena | Institute of Solid State Physics, Friedrich Schiller University Jena | Institute of Solid State Physics, Friedrich Schiller University Jena | Institute of Solid State Physics, Friedrich Schiller University Jena | Institute of Solid State Physics, Friedrich Schiller University Jena | Institute for Chemical Research, Kyoto University | Institute of Solid State Physics, Friedrich Schiller University Jena | Institute for Chemical Research, Kyoto University | Institute of Solid State Physics, Friedrich Schiller University Jena | Institute for molecular science

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: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: ARPES, TMDC, organic molecule

A chirality-induced spin-selective (CISS) effect with controlled chiral molecules on various solid surfaces has been actively studied for applications in spintronics, enantioseparation, and other areas [1]. However, many aspects of this phenomenon, including its mechanism of the extraordinal large CISS, remain unknown.

Our approach to this challenge is to fabricate a well-defined surface chirality system on solid surfaces with well-established electronic spin band structures and an oriented chiral molecule, investigating how the surface chirality affects the emitted electrons from the solid by measuring the momentum-resolved photoelectron. Hence, the electron scattering effects of the surface chirality on the CISS by evaluating changes in the substrate band structure before and after the adsorption of the chiral molecule would be studied.

In this study, the enantiopure chiral molecule thiadiazole-[9]helicene (TD[9]H) [2] was used, where TD[9]H is a [9]helicene terminated with a five-membered ring containing nitrogen and sulfur. The substrate is a monolayer WS$_2$/Au(111) (ML-WS$_2$) with spin-polarized bands (bands at ’ and points) showing symmetrical dispersion across the point [3]. After depositing the enantiopure TD[9]H on the ML-WS$_2$ under ultra-high vacuum condition, the surface chirality was measured by low-energy electron diffraction (LEED), where the right-/left-handed chiral molecular films exhibited no mirror plane respectively but showed the mirror inversion relationship with each other. The results taken by angle-resolved photoelectron spectroscopy (ARUPS) will be discussed by comparing the changes of ’ and -point bandwidths of ML-WS$_2$ before and after molecular adsorption.

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Impacts of interfacial modifications on functionalities of organic semiconductors

by Kouki Akaike | National Institute of Advanced Industrial Science and Technology

Abstract ID: 10420
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: graphitic carbon nitride, interfaces, organic semiconductors, organic solar cell, photoelectron spectroscopy, work function

Applications of organic semiconductors to electronics and energy harvesting generally involve multi-stacked layers of both organic and inorganic materials. Interfaces of dissimilar materials play decisive roles in determining their functionality, performance, and stability in practical use. Understanding and controlling energetic landscapes and interfacial structures is thus critical for reasonably designing interfaces and optimizing the performances of envisioned applications.

Among multiple interfaces, organic/metal interfaces govern the charge injection and extraction processes between an organic semiconductor and an electrode. One of the critical parameters determining these processes is the work function (WF), which determines the energetic barrier height at the interfaces in the elementary charge processes. We will present the control of electrode WFs with a relatively air-stable donor and a molecule that plants bio-synthesize. Organic/organic interfaces affect the charge generation and injection/extraction in solar cells and light-emitting diodes, respectively. We will secondly introduce the study on the impact on the performance of organic solar cells by modulating the molecular orientation of an acceptor. We will finally move on to the topic of an emerging organic photocatalyst, graphitic carbon nitride, g-CN. The film of this visible-light-driven photocatalyst can be deposited on a substrate and chemically modified by the substrate surface. We report that the chemical modifications of g-CN films with soda glasses promote photocatalytic reactions due to the facilitated charge separation induced by introducing electron-withdrawing groups into g-CN.

Insight into the charge transport mechanisms of molecular crystals

by Satoshi Kera | Keisuke Fukutani | Institute for Molecular Science | Institute for Molecular Science

Abstract ID: 10328
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Photoelectron spectroscopy, band dispersion, electron-phonon coupling, rubrene single crystal

Understanding the impacts of weak electronic interaction on the electron delocalization is required to unveil the rich functionalities and mysterious properties of organic molecular materials. Moreover, the temporal and spatial effects of the strong coupling of phonon (collective lattice vibration) and/or local molecular vibration to electron must be discussed. Angle-resolved ultraviolet photoelectron spectroscopy (ARUPS) is known to be a powerful technique to study the valence electronic structure. The frontier orbital of HOMO state can offer a wide variety of key information, that is essential to comprehend charge-hopping transport (small-polaron related transport) in the ordered monolayer film [1] as well as to coherent band(-like) transport in the molecular single crystal [2,3]. However, the experimental study of ARUPS fine features of the HOMO state has not been progressed till recently due to difficulty in the sample preparation, charging effects, irradiation damages, and so on [4,5]. We present the latest development for the ARUPS measurements of electronic states of rubrene ($C_{42}H_{28}$) single crystal by using low-energy excited and high-resolution experimental station at BL7U of UVSOR synchrotron facility. We demonstrate how the HOMO band is observed differently against the previous results in theory [6] for the orthorhombic crystal structure of rubrene. The precise experiments of the temperature and photon energy dependences of 2D momentum-energy scanning for the ARUPS shed light on the problem of describing the characteristics of the electronic structure of organic crystals [7], and thus the results would provide a perspective for the design of organic semiconductor devices.

In-situ controlled nucleation of organic single crystal arrays via femtosecond laser-induced

by Zhi-Kun Ji | Yue-Feng Liu | Jing Feng | College of Electronic Science and Engineering, Jilin University | College of Electronic Science and Engineering, Jilin University | College of Electronic Science and Engineering, Jilin University

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: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Femtosecond laser, In-situ controlled nucleation, Organic semiconductor single crystals

Organic semiconductor single crystals (OSSCs), due to the long-range ordered arrangement of molecules, absence of grain boundaries and low content of impurities, are widely used in organic light-emitting diodes (OLEDs), organic field-effect transistors (OFETs) and organic photodetectors (OPDs). Due to their achievable flexibility and cost-effective solution processing, they are considered to have great potential in the consumer electronics market. However, in traditional solution-based process preparation, crystal nucleation in solution is often dominated by solvent evaporation, and the stochastic nucleation processes in solution makes controlled nucleation growth of crystals still challenging. Here, we propose a photothermal convection-dominated femtosecond laser-induced nucleation strategy. By introducing silver as a photothermal substrate, the thermal gradient generated by femtosecond laser irradiation of the silver substrate is used as a driving force to generate convection-induced aggregation of organic molecules and induce nucleation. By adjusting the laser parameters, the convection intensity and aggregation time can be varied to regulate the number of crystal nuclei, thus enabling in-situ growth and controlled preparation of organic single crystals. The laser-induced organic single crystals have good surface morphology and homogeneous fluorescence luminescence properties. the crystal stacking pattern and fluorescence spectra of the laser-induced crystal are consistent with those of naturally crystalline crystals, demonstrating that this is non-photochemically induced nucleation (NPLIN) process. Based on the processing flexibility and template-free processing of femtosecond laser writing, highly crystalline organic semiconductor single-crystal arrays with different patterns can be prepared without any template assistance, and the controlled growth of single crystals can be achieved by multiple dropwise solution injection. This provides a flexible and precisely controlled nucleation strategy for the preparation of organic semiconductor single-crystal arrays, thus offering a new way for the preparation of arrayed optoelectronic devices.

Interface material design for efficient and stable organic solar cells

by Xiangjian Wan | Nankai University

Abstract ID: 10501
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Organic solar cell, efficiency, interface layer, stability

It remains a formidable challenge for achieving efficient and stable organic solar cells (OSCs). Just recently, we have designed and developed a type of 1,8-naphthalimide dicarboxylic acid interface modification material. Through the interaction of dicarboxylic acid and zinc oxide as the electron transport layer material, a hybrid electron transport layer was formed, which could simultaneously improve the efficiency and stability of the inverted structure OSCs. The above-mentioned interface modification materials had considerable thickness tolerance and could be used not only for small area devices, but also for preparing large-area modules. In addition to being suitable for modifying zinc oxide interface materials, the devices prepared using modified SnO2 interface also showed high efficiency and good stability. Furthermore, flexible and stable OSCs based on the above interface materials were fabricated and showed impressive efficiency and good flexible properties.

Investigation on hole transfer dynamics during charge separation process in non-fullerene organic solar cells

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: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: organic solar cells; non-fullerene acceptor; charge transfer state; hole transport; energy loss

In the conventional fullerene-based organic photovoltaics (OPVs), in which the excited electrons from the donor are transferred to the acceptor, an electron charge transfer state (${}^{e}E_{\mathrm{CT}}$) that electrons pass through has a great influence on the device performance. In the bulk-heterojunction (BHJ) system based on low band-gap non-fullerene acceptor (NFA), however, a hole charge transfer state (${}^{h}E_{\mathrm{CT}}$) from the acceptor to the donor has a greater influence on the device performance. The accurate determination of the ${}^{h}E_{\mathrm{CT}}$ is essential for achieving further enhancement in performance of non-fullerene organic solar cells. However, the method for determining the exact ${}^{h}E_{\mathrm{CT}}$ remains an open challenge. Here, we suggest a simple method to determine the exact ${}^{h}E_{\mathrm{CT}}$ level by deconvolution of EL spectrum of BHJ blend ($\mathrm{EL_B}$). To generalize, we have applied our $\mathrm{EL_B}$ deconvolution method on nine different BHJ systems consisting of the combination of three donor polymers (PM6, PBDTTPD-HT, PTB7-Th) and three NFAs (Y6, IDIC, IEICO-4F). Under the conditions that (i) absorption of the donor and acceptor are separated sufficiently, and (ii) the onset part of the external quantum efficiency (EQE) is formed solely by the contribution of the acceptor only, $\mathrm{EL_B}$ can be deconvoluted into the contribution of the singlet recombination of the acceptor and the radiative recombination via ${}^{h}E_{\mathrm{CT}}$. Through the deconvolution of $\mathrm{EL_B}$, we have clearly decided which part of the broad $\mathrm{EL_B}$ spectrum should be used to apply the Marcus theory. Accurate determination of ${}^{h}E_{\mathrm{CT}}$ is expected to be of great help in fine-tuning the energy level of donor polymers and NFAs by understanding the charge transfer mechanism clearly.

Lattice Battery Solar Cells —Exceeding Shockley-Queisser Limit

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Abstract ID: 10290
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Shockley-Queisser limit, gold triangle of solar cells, lattice battery solar cells, lattice energy reservoir

Due to the extremely broad solar spectral distribution and the fixed bandgap of absorbers in single-junction solar cells, the theoretical efficiency of solar cells is limited to less than 33%, referred to as the Shockley-Queisser (SQ) limit for single junction solar cells.[1] In other words, around 70% of the solar energy cannot inherently be converted into electricity even with perfect fabrication. Two major energy losses include, (1) hot carriers photogenerated by high energy photons losing their extra energy through ultrafast thermalisation (cooling) and lattice heating. (2) sub-bandgap photons (typically infrared) not being absorbed due to an extremely low absorption coefficient.

A revolutionary concept of lattice battery solar cell (LBSC) is proposed to leap the conversion efficiency by inherently eliminating two major energy losses of conventional solar cells, namely hot carriers and non-absorption of the substantial near infrared (NIR) emission. In an LBSC, hot phonon emission will be saved into lattice energy reservoir through electron-lattice coupling; NIR solar emission is harvested by a NIR-perovskite composition. The NIR-generated carriers are upconverted to the conduction band (CB) of perovskites driven by lattice energy reservoir. The theoretical efficiency of LBSCs is estimated to be over 70%, significantly exceeding the Shockley-Queisser limit. In addition, LBSCs have lower operational temperature thus much improved stability due to eliminating heating source from hot carriers. Different from the existing multijunction solar cells, LBSCs will keep the single layer structure with low-cost fabrication. Therefore, LBSCs could perfectly satisfy the golden triangle of solar cell performance, which prospects great competitive advantage for further commercialization.

lead-free perovskite and photovoltaic devices

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Abstract ID: 10312
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Lead-free perovskite, Photovoltaic device, Solar cell

Perovskite solar cells (PSCs) have attracted broad attention. The certified efficiency has exceeded 26%, which is comparable to silicon-based counterparts. However, the environmental problems caused by the lead in perovskite restrict their large-scale applications.

If a monovalent metal ion and a trivalent metal ion are used instead of two lead ions, a double perovskite A2M+M3+X6 is realized. In order to resolve toxicity of lead-based perovskites, Bo Qu group prepared PSCs based on lead-free double perovskite Cs2AgBiBr6 in 2017 (Adv. Sci. 2018, 5, 1700759), and then fabricated semi-transparent solar cells with an average visible light transmittance of 73% (Sol. RRL 2020, 4, 2000056).

However, the relatively large bandgap (~2.0 eV) of Cs2AgBiBr6 hinders its optoelectronic applications in longer wavelength bands of visible and near-infrared regions. We replaced some of Bi elements in Cs2AgBiBr6 with trace doping (~1%) of iron (Adv. Function. Mater. 2021, 322109891) and ruthenium (Mater. Adv. 2022, 3, 4932) to broaden its absorption range to near-infrared region (1200-1350 nm). The above single crystal materials exhibit excellent near-infrared light detection. And we were invited to write a review article (J. Phys. Chem. Lett. 2023, 14, 5310).

At present, the photovoltaic performance of lead-free perovskite still does not meet theoretical expectations. We have summarized the problems that exist in different lead-free perovskites (Mater. Today Energy 2018, 8, 157; Adv. Energy Mater. 2019, 1902496) and these limitations were mainly ascribed to low carrier transport and self trapping effects caused by low structural or electronic dimension of lead-free perovskites, as well as the non-radiative recombination. The bottleneck in the application of lead-free perovskite photovoltaics can be overcome by regulating the structural or electronic dimensions, and we were invited to publish a cover article in Chemical Society Reviews (2024, 531769-1788) entitled "Breaking the Bottleneck of Lead Free Perovskite Solar Cells through Dimensional Modulation".

Light Manipulation in Organic Light-Emitting Devices by Using a Bifunctional Meta-Electrode

by Jing Feng | Jilin University

Abstract ID: 10489
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Light manipulation; Organic light-emitting devices; Meta-electrode

Organic light-emitting devices (OLEDs) with polarized and directional emission are highly desired for their promising applications in optical imaging, optical communication, and immersive visual technologies. Existing implementation methods based on free space bulk optical elements suffer from significant power loss, limiting their practical applications. Here, a bifunctional meta-electrode is proposed by integrating a metasurface consisting of Ag periodic corrugations onto the ITO anode to simultaneously realize the functions of charge carrier injection and photon management in the OLEDs. Highly polarized and directional light emission is demonstrated while maintaining a high device efficiency using the meta-electrode. The electroluminescence with a polarization extinction ratio of 5 is achieved by judiciously engineering the polarization-dependent Purcell factor of the resonant cavity constructed by the meta-electrode. Meanwhile, the directional light emission with a divergence angle of 10° can be obtained by the efficient out-coupling of surface plasmon-polariton mode. The light beam can be collimated in one direction by using 1D nanogratings and in two directions by using 2D nanopillars, respectively.

Light-emitting radicals and their devices

by Feng Li | Jilin University

Abstract ID: 10008
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: light-emitting materials; luminescent radicals; doublet emission; OLEDs; radicals

Due to the single unpair electron in mono-radicals, the spin configurations of their excited states and ground state are both doublets. So, the emission process is spin-allowed. We exploited a light-emitting radical, TTM-1Cz, as the emitter to fabricate the first OLED with doublet emission.[1] The problem caused by the spin-forbidden transition of triplet exciton in traditional fluorescent OLEDs is circumvented. After continually optimizing materials and device, a D-A type luminescent radical emitter, TTM-3NCz, was used as the emitter of an OLED with a maximum external quantum efficiency of 27 %, and the first-excited state is thought to be a charge-transfer doublet state.[2] Through exploiting a TADF host, the energy transfer from singlet and triplet excitons to doublet excitons was confirmed and the efficiency roll-off was improved.[3]

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Luminescence of the Molecules with Double Excitation Character

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Abstract ID: 10304
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: double excitation; delayed fluorescence; singlet; triplet

In molecular excited states, energy level of S1 is higher than that of T1, because of the exchange energy of two electrons in the excited state. Leupin et al. reported that azaphenalene molecules have un-overlapped HOMO and LUMO and may show negative ΔEST (E(S1) – E(T1)), based on energy transfer experiments and short T1 lifetime (0.1 µs).[1] Domcke et al. reported that the heptazine molecules showed negative ΔEST in wave function-based quantum chemical calculations, and the spectroscopic absence of T1 state indicating the negative ΔEST.[2]

We designed and synthesized the heptazine molecules showing negative ΔEST of –11 meV.[3] The energy inversion of the S1 and T1 excited states results in delayed fluorescence with short lifetime of 0.2 µs, decreasing with decreasing temperature. OLEDs using this molecule exhibited a fast transient electroluminescence decay and a high external quantum efficiency of 17%.

There have been many reports on computational design of the molecule for negative ΔEST, but the molecular structures have been limited to the B/N-introduced azaphenalene-type structures, except a few reports on some alternant hydrocarbon molecules.[5] For negative ΔEST, the exchange interaction should be as small as possible and S1 must be stabilized more than 2·K. When the S1 state have the multi electron configuration mixed with the double excitation character, it can be more energetically lowered than T1. We computationally designed and proposed the linearly extended BN ladder-type molecules[4], for which the negative ΔEST and large oscillator strength were estimated by double hybrid TD–DFT calculations with B2PLYP and SOS-PBE-QIDH functional.

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Micro/nano-structured metallic electrodes in Organic light-emitting devices

by Yan-Gang Bi | Jing Feng | Jilin University | Jilin University

Abstract ID: 10507
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: OLED, light manipulation, metasurface, micro/nano-structure

Organic light-emitting devices (OLEDs) have been widely used in flat panel displays and solid-state lightings, benefiting from their excellent characteristics of self-emitting, wide viewing angle, high luminous efficiency associated with low power consumption, high contrast and fast switching speed. OLEDs with polarized and directional light emission have many practical applications, however, beam shaping of these devices is fundamentally challenging because they are Lambertian light sources. On the other hand, low light extraction efficiency of OLEDs is also a main bottleneck. Around 80% of internally generated photons is trapped in forms of waveguide modes, surface plasmon-polariton mode, and substrate mode.

Optical metasurfaces with micro/nano patterns have provided new opportunities in designing ultrathin and compact optical and optoelectronic devices due to their capabilities for unprecedented control over the wavefront, phase, polarization, and amplitude properties of light in a desired manner. Here, we proposed meta-electrodes by integrating metallic metasurfaces with electrodes to manipulate photons in OLEDs. Non-radiative modes in OLEDs have been effectively excited and outcoupled with obvious improvements in luminance and external quantum efficiency. In addition, the linearly polarized emission with a high polarization ratio and directional emission at a desired angle have been demonstrated in OLEDs based on light manipulation induced by the optical metasurfaces.

Molecular Carbons with Different Topologies: Synthesis, Electronic Properties and Open-Shell Singlet Diradical Ground States

by Chunyan Chi | Department of Chemistry, National University of Singapore

Abstract ID: 10431
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Materials design and synthesis, Processing and structural characterization, Spin and magnetism

Carbon-based nanostructures have shown revolutionary influence in the area of chemistry, physics and materials science. Recent efforts have been focused on novel topological structures of sp2-carbons such as carbon nanohoops, nanobelts, molecular cages, and open-shell nanographenes, which provoked new chemistry and materials. However, synthesis of this kind of molecules is extremely challenging mainly due to strain or intrinsic high reactivity. Another issue is that most of these carbon nanostructures have a localized aromatic character; that means, the π-electrons are not globally delocalized along the backbone, which limits their optical and electronic properties and applications. Herein, synthesis of a series of novel pi-structures with different topologies will be introduced (Figure 1), and their physical properties, aromaticity, diradical character and applications will be discussed.[1-8]

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Molecular Orientation at Organic semiconductor/Dielectric Interfaces and their OFET Device Characteristics

by Takayuki Miyamae | Chiba University

Abstract ID: 10496
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: interface, morecular orientation, organic-field effect transistor, sum frequency generation

Organic field-effect transistors (OFETs) are promising for key components of flexible devices. Although organic semiconductors with high charge mobility and atmospheric stability have been actively developed, ambipolar organic semiconductors are essential for the fabrication of integrated microelectronic organic circuits and optoelectronic devices. Indigo, a natural dye derived from plants, exhibits well-balanced ambipolar organic semiconducting properties when the insulating passivation layer is underlying [1]. In this study, the effects of the molecular orientation of an insulating tetratetracontane (TTC) interlayer on the crystallinities of the semiconducting layers deposited on top and the electrical properties of the OFETs were investigated by sum-frequency generation (SFG) spectroscopy [2]. The insulating interlayer significantly increased the crystallinity of the semiconducting indigo when the thin TTC film annealed at 70 °C was used. Electronic SFG revealed that the crystallinity at the indigo interface was also enhanced by the low-temperature annealing of TTC, indicating the importance of controlling the molecular orientation of the underlying molecular layer for improving the performance of OFETs. In vibrational SFG, the molecular orientation of the underlying TTC was disrupted by the stacking of the semiconducting layer. Although the orientation can be significantly improved via low-temperature annealing of the TTC layer, we consider that this disturbance in the molecular orientation is caused by stacking stresses. Hence, the stacking-stress effect and the disruption of the molecular orientation are important issues that must be considered in constructing devices using organic semiconductors.

In this presentation, I will also address some other topics related to the relationship between molecular behavior at the organic semiconductor/insulator interface of OFETs and OFET properties.

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M-series nonfullerene acceptors for polymer solar cells

by Qingdong Zheng | Nanjing University

Abstract ID: 10355
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Organic semiconductors; Polymer solar cells; Nonfullerene acceptors; Molecular orientation

Control over the intermolecular interaction as well as the molecular orientation of organic semiconductors with respect to the substrate plays a critical role in determining the performance of polymer solar cells (PSCs). In this talk, we will focus on the development of novel electron-transporting materials based on ladder-type heteroheptacenes without sp^3-hybridized carbons for efficient PSCs. A series of ladder-type heteroheptacene-based small molecules with branched or unbranched side chains flanked in different positions of their conjugated backbone, or with varied electron withdrawing end groups flanked on the same conjugated backbone, were designed and synthesized to investigate the effect of side-chains and end group on the crystallinity, molecular orientation, charge transport and photovoltaic properties of these ladder-type heteroheptacene-based semiconductors. Furthermore, we report the effect of noncovalent intramolecular interactions on the photovoltaic performance of the nonfullerene acceptors. The removal of the sp^3-hybridized carbons leads to novel nonfullerene acceptors with efficient electron transport. As results, the best-performance nonfullerene acceptor with optimized molecular orientation affords an outstanding power conversion efficiency of over 18%.

Multimode optical switch based on polymer waveguide

by Xibin Wang | Shijie Sun | Xiaoqiang Sun | Fei Wang | Fei Wang | Jilin University | Jilin University | Jilin University | Jilin University | Jilin University

Abstract ID: 10518
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Mode-division multiplexing, Multimode optical switch, Polymer waveguide

Multimode optical switch is becoming more and more important as one of the key elements for mode-division multiplexing (MDM) optical communication systems. However, the different structural relationships between the waveguides and the different modes make it challenging to control more spatial modes flexibly. Here, we propose and experimentally demonstrate a dual-mode optical switch on polymer waveguide platform, which could realize arbitrary combinations of unitary transmission matrices of E_{11} and E_{21} modes and also greatly reduce the power-consumption. For the proposed dual-mode optical switch, three asymmetric Y-junctions are used as mode (de)multiplexers, two Mach-Zehnder interferometers form a single-mode switch matrix, and a 2×2 multimode interferometer is used as the waveguide crossing. We fabricated the device with simple photolithography and wet-etching methods. Our fabricated device based on polymer waveguide platform shows a low power-consumption. The proposed device can greatly improve the flexibility and efficiency of reconfigurable MDM networks.

Multiple-Temporal Scale Exciton Dynamics in Organic Photovoltaics

by Kangning Zhang | Shandong University

Abstract ID: 10522
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: exciton dynamic, organic solar cells, photovoltaic stability

Benefiting from the synergistic development of material design, device engineering, and the mechanistic understanding of device physics, the certified power conversion efficiencies (PCEs) of single-junction non-fullerene organic solar cells (OSCs) have already reached a very high value of exceeding 20%. This progress provides an opportunity for their commercial application to be within sight. The fundamental photo-to-electricity conversion theory concerns a series of exciton and charge dynamic processes in the timescale ranging from femtoseconds to microseconds. Clearly revealing these kinetic processes is the key to improve device PCEs, understand the operating principles, and enhance photovoltaic stability. Although the framework for describing both exciton and charge dynamics of OSCs has been preliminarily established, some surprising and controversial theoretical and experimental observations still need more investigations. Especially, the dynamic parameters of charge recombination, trap-state response, and the kinetic evolution information associating with stability should be highlighted in state-of-the-art non-fullerene-based OSCs. In this report, we will discuss and analyze the detailed evolution of excitonic and electronic excitations, and the photophysical property-function relationship in state-of-the-art OSCs. It would further help to recognize and understand the essential mechanisms of the present and potential problems of the cells and to explore approaches for solving them.

Near-infrared and visible light dual-mode Organic Photodetectors and Applications

by Furong Zhu | Hong Kong Baptist University

Abstract ID: 10323
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: NIR, Organic photodetector, dual-mode, multispectral detection, photoresponse

Organic photodetectors (OPDs) are a promising alternative optical detecting technology to conventional wafer-based inorganic counterparts, because the optical and electric properties of the organic semiconductor materials can be tailored accordingly. They offer additional advantages such as having a solution-processable fabrication process, which also leads to significant cost benefits, thereby creating next-generation solution-processable, flexible, and low-cost photodetectors. In general, the spectral responses of the photodetectors are determined by the absorption of the active materials and optical profile in the devices. Single-band OPDs optimized for photodetection at specific spectral ranges have been reported. However, the reports on OPDs for multispectral detection are rather rare. It is a great challenge to achieve high-performance multispectral OPDs.

This talk discusses the performance of novel near-infrared (NIR) and visible light dual-mode OPDs. The NIR/visible light dual-mode OPD also allows multispectral detection that is controlled by the polarity of a bias applied between the two contacts in the device. The OPD also exhibits a broadband photoresponse when it is operated using a 50% duty-cycled square-wave voltage supply [1-5].

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Nonequivalent hybridization generated lone pairs inside charge transfer cocrystals modifying spin resonance and the intersystem crossing between singlets and triplets

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Abstract ID: 10562
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: electron-phonon coupling, lone pairs, nitrogen substitution, spin-orbital coupling

Lone pairs are widely prevalent in various types of molecules and have significant impacts on the material's band structure, transport properties, dielectric response, among others. Extensive research has been conducted on the role of lone pair electrons in materials such as perovskites and topological quantum materials. Herein, we fabricated three charge transfer cocrystals containing 0, 1 and 2 nitrogen atoms in the donor and conducted a detailed investigation on the effects of nonequivalent hybridization generated lone pairs in pure organic small molecule cocrystals.

Firstly, the introduction of lone pairs or nitrogen substitution alters the electrostatic potential distribution of the donor, thereby influencing the interaction between the donor and acceptor. Single-crystal X-ray diffraction results indicate that with an increase in the number of nitrogen substitutions, the distance between donors and acceptors enlarges, resulting in a decrease in the high-frequency dielectric constant and a shorter lifetime of electron-hole pairs. Furthermore, the introduction of lone pairs could enhance the spin-orbit coupling (SOC). Combining with theoretical calculations, we found that lone pairs can adjust the spin density distribution within the system through SOC and enhance symmetry breaking. With SOC as the medium, the introduction of lone pairs also augments the interaction between the spin and lattice, leading to a more pronounced enhancement of the electron paramagnetic resonance (EPR) signal under illumination as the number of lone pairs increases. Lastly, due to the modifications in spin-orbit coupling and the lifetime of electron-hole pairs induced by the introduction of lone pairs, the system exhibits diverse optical phenomena under an external magnetic field.

Overall, the introduction of lone pairs through nonequivalent sp2 hybridization significantly impacts the spin and dipole properties of cocrystals, offering valuable insights for the synthesis of functional crystalline materials.

Novel strategies in printable photon-upconversion, OLEDs and wearable electronics

*by Le Yang | IMRE, A*STAR*

Abstract ID: 10356
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: OLEDs, TTA-upconversion, organic electronics, organic semiconductors, triplet-triplet annihilation

Triplet-triplet annihilation (TTA) enables efficient and versatile photon-upconversion in organics. The same process also can enhance OLED efficiencies by utilising dark triplets.[1-4] Here, we present progresses on efficient TTA-UC in novel composite systems[5-6]:

First, we use a hybrid nanocrystal as triplet-sensitizer, and two different organic upconversion emitters, we observe for the first time, a multi-fold enhancement in the upconversion efficiency in such a composite hybrid system.[5]

Next, solid-state photon-upconversion always suffers from low efficiencies and high threshold excitation power. We showcase a novel composite-sensitizer, inspired by the BHJ donor-acceptor of organic photovoltaics, for TTA-UC devices, leading to highly-efficient solid-state upconversion devices with low excitation power, through a one-step solution method. We also scaled-up this strategy on highly-flexible large-area substrates.[6]

Lastly, we explore overcoming the efficiency bottleneck in simple fluorescent OLEDs. First, in a dual-dopant system, lifting rubrene-derivative-based OLEDs to >20% EQE.[1-2] Secondly, in single-dopant devices, by triplet-fusion mechanism, drawing parallels to TTA-UC, to enhance device efficiency ceiling.[3-4]

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Octahedron distortion-triggered dipole–spin interaction in multiferroic magnetoelectric perovskites

by Xiangqian Lu | Wei Qin | School of Physics, Shandong University | School of Physics, Shandong University

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: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Organic-inorganic hybrid perovskite; multiferroic; magnetoelectric coupling; magneto-optic effect; dipole–spin interaction

The design of perovskite structures with multiferroic magnetoelectric coupling effects opens up new opportunities in fields such as the creation of next-generation spin-dependent multistate information storage technologies. In this work, we prepared a transition metal-implanted perovskite with multiferroic magnetoelectric coupling, in which both magnetoelectric coupling and a blueshift of photoluminescence were observed. Combining theoretical simulation and experimental data shows that the interstitial implantation of metal atoms does not destroy the periodic structure, but the octahedron is distorted.The introduction of transition metal-generated polarized spin interacts with the electronic orbit through spin–orbital coupling to lead to a pronounced octahedron distortion, where the temperature dependence of the dielectric constant undergoes a ferroelectric polarization transition. An external magnetic field could enhance the strength of spin polarization to further affect the magnitude of electric polarization. Moreover, applying an electric field tunes the distortion of the octahedron dependence of electric polarization to feed back to the change in spin polarization. Overall, the spin polarization-induced electric polarization in perovskites provides a unique approach to realizing the room temperature magnetoelectric coupling of multiferroic materials.

Optical Modeling of OLEDs with Non-uniform Layers Based on Single Surface Approximation

by Linya Chen | Honggang Gu | Xiaoke Guo | Shiyuan Liu | Huazhong University of Science and Technology | Huazhong University of Science and Technology | Huazhong University of Science and Technology | Huazhong University of Science and Technology

Abstract ID: 10147
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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Non-uniform Layers, OLED, Optical Modeling, Single Surface Approximation

Inkjet-printed processing technology (IJP) has recently been implemented to manufacture OLED displays. Compared with evaporation, IJP does not need a fine metal mask (FMM) and has the advantages of high material utilization, large area, low cost, and flexibility, which is the trend of future display processing. However, the coffee ring effect (CRE) is an inevitable phenomenon in IJP, leading to non-uniform thickness and affecting device performance[1]. Up until now, most OLED optical models have assumed that the thickness is uniform and rarely consider the situation that the thickness is non-uniform.

In this paper, an optical model based on single surface approximation is proposed to simulate the properties of OLEDs with non-uniform layers. First, considering that the light radiated by each dipole is incoherent, the OLED is divided into several regions according to the radiation range of each dipole. Then, each region is subdivided into M equal fractions, and each slice is assumed to be distributed in parallel. It is worth noting that each fraction's thickness and incidence angle should be modified according to the non-uniform layer's actual thickness and surface morphology[2-3]. The optical characteristics of each film are measured by a spectroscopic ellipsometer (ME-L, Wuhan Eoptics Technology Co.). The consuming time is reduced by about five times compared to traditional models such as FEM and FDTD.

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Organic electrochemical transistors with electroactive composite films based on nature-derived matrix materials

by Felix Sunjoo Kim | Chung-Ang University

Abstract ID: 10195
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: cellulose, coating, composite film, electrochemical transistor

We present organic electrochemical transistors with electroactive composite films based on a cellulose matrix. Cellulose derivatives can act as a structural matrix when blended with polymers or ionic molecules in composite films. The composites are easily processable with solution-based technology to form excellent thin films. We show that the composites with cellulose matrix can enable an efficient transport of charge carriers. The composite films are then employed as various active components in organic electrochemical transistors. The relationships between structure, composition, processing, and performance are studied. We also present our current effort to diversify technological approaches for enhancement of device performance and to seek nature-derived materials as an active component in organic transistors for sustainable development.

Organic Microlaser Materials and Devices

by Yong Sheng Zhao | Institute of Chemistry Chinese Academy of Sciences

Abstract ID: 10240
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Organic optoelectronics; organic laser; laser display; photonic skin

Exploring a universal technique for the manufacture of reproducible organic material geometries in large quantities, just as photo-lithography is to the traditional silicon-based electronics and photonics, is essential for the upcoming flexible integrated photonics. We developed a solution printing strategy for the function-directed controllable and rapid fabrication of high-quality organic microlaser arrays, which was subsequently applied as the building blocks of the panels of organic laser displays and as the elements if photonic integrated circuits. The printed soft photonic systems show competitive performances with their nowadays silicon-based counterparts; and moreover, they even take advantages of mild processing, flexible doping, active/responsive characteristics, etc.

Organic Single-Crystalline Semiconductor Thin Films for Light-Emitting Devices

by Ran Ding | Jilin University

Abstract ID: 10487
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: organic single-crystalline semiconductor; OLEDs; organic single crystals; single-crystalline thin films

Since the first observation of electroluminescence from anthracene single crystals in 1963 by Pope et al., organic single-crystalline semiconductors constructed by π-conjugated molecules have attracted great attention due to their unique and superior features for optoelectronic applications. Their inherent long-range molecular ordering provides a great opportunity for fundamental research on the basic molecular interactions and structure-property relationships. The regular and dense packing of molecules contributes to the high mobility of charge carriers, and oriented alignment of transition dipole moments, which is conducive to optoelectronic devices achieving fast exciton formation and high light outcoupling. Specially, the highest mobility of 43 $cm^2 V^{-1} s^{-1}$ has been recorded by a double-gate field-effect transistor based on rubrene single crystals. Via the rational molecular design and crystal engineering, the luminescence efficiency of organic single-crystalline semiconductors has exceeded 80%. Further advantages of organic single-crystalline semiconductors are their low impurity level, high thermal stability, and large refractive indices, as well as amplified spontaneous emission (ASE) phenomenon giving rise to a spectrally narrowed emission. Encouraged by these impressive findings, organic single-crystalline semiconductor thin films have been considered as an ideal candidate for constructing high-performance solid-state light-emitting devices. Over the past decade, great efforts have been devoted by our group to the development of single-crystal OLEDs for realizing bright and efficient EL emission. The realization of three-primary-color and white single-crystal OLEDs with improved EL performances constituted a major step toward practical flat-panel display and solid-state lighting applications.

Organic Single-Crystalline Semiconductor Thin Films for Light-Emitting Devices

by Ran Ding | Jilin University

Abstract ID: 10490
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: organic single-crystalline semiconductor; OLEDs; organic single crystals; single-crystalline thin films

Since the first observation of electroluminescence from anthracene single crystals in 1963 by Pope et al., organic single-crystalline semiconductors constructed by π-conjugated molecules have attracted great attention due to their unique and superior features for optoelectronic applications. Their inherent long-range molecular ordering provides a great opportunity for fundamental research on the basic molecular interactions and structure-property relationships. The regular and dense packing of molecules contributes to the high mobility of charge carriers, and oriented alignment of transition dipole moments, which is conducive to optoelectronic devices achieving fast exciton formation and high light outcoupling. In particular, the highest mobility of 43 cm^2 V^{-1} s^{-1} has been recorded by a double-gate field-effect transistor based on rubrene single crystals. Via the rational molecular design and crystal engineering, the luminescence efficiency of organic single-crystalline semiconductors has exceeded 80%. Further advantages of organic single-crystalline semiconductors are their low impurity level, high thermal stability, and large refractive indices, as well as amplified spontaneous emission (ASE) phenomenon giving rise to a spectrally narrowed emission. Encouraged by these impressive findings, organic single-crystalline semiconductor thin films have been considered an ideal candidate for constructing high-performance solid-state light-emitting devices. Over the past decade, great efforts have been devoted by our group to the development of single-crystal organic light-emitting devices (OLEDs) for realizing bright and efficient EL emission. The realization of three-primary-color and white single-crystal OLEDs with improved EL performances constituted a major step toward practical flat-panel display and solid-state lighting applications.

Organic Thin Films-based Photovoltaics for Indoor Operation

by Jae Won Shim | Korea University

Abstract ID: 10030
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: indoor operation, organic thin film, parasitic resistance, photovoltaic

With the advent of autonomous low-powered indoor electronic devices such as wearable devices, or wireless sensor nodes for the Internet of Things (IoT), the need for new types of energy harvesting systems without further replacement or maintenance is increasing day by day. Among many candidates, organic photovoltaics (OPVs) have been considered as one of the most promising energy sources due to their optical, mechanical, and electrical properties such as tunable absorption range, mechanical flexibility, light in weight, *etc*. In this talk, our recent research work related to advances of the photovoltaic performance of OPVs for indoor operation (under light emitting diodes (LEDs), fluorescent light, halogen lamp, etc. conditions) is presented. In particular, we maximized the device performance through the optimization of parasitic resistance effects associated with charge-collecting electrode, interlayers and photoactive layers of the OPVs. This talk discusses different types of strategies for the efficient indoor OPVs including un-doped ZnO films for transparent electrodes, polymer surface modification, ultra-thin ITO, oxide/metal/oxide (OMO) electrodes.

Photoemission Angular Distribution (PAD) of Well-Ordered DPh-BTBT Films - Origin of Mixed-Orbital Carrier Transport

by Yoichi Yamada | Yutaro Ono | Ryohei Tsuruta | Yuri Hasegawa | Hiroyuki Ishii | Univ. of Tsukuba | Univ. of Tsukuba | Univ. of Tsukuba | Univ. of Tsukuba | Univ. of Tsukuba

Abstract ID: 10436
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Organic Semiconductors, Photoemission, Photoemission Angular Distribution, Scanning Tunneling Microscope

Recently, in certain high-mobility organic semiconductors, mixed-orbital carrier transport, a phenomenon in which multiple frontier orbitals of molecules are involved in carrier conduction, has been noted. Although this phenomenon has been studied theoretically, there has not yet been experimental research from the viewpoint of direct measurements of the electronic structure of thin films. Here, we studied the origin of mixed-orbital carrier transport in BTBT molecules by precisely measuring the electronic states of the well-ordered films of DPh-BTBT.　We used scanning tunneling microscopy, synchrotron radiation photoemission spectroscopy, and photoelectron tomography to focus on the shape of the molecular orbitals in the thin films.

In the highly oriented DPh-BTBT thin film, the photoemission angular distribution (PAD) of HOMO and HOMO-1 showed a similar pattern due to the similar shape of these wavefunctions. In addition, first-principles calculations confirmed the hybridization of HOMO and HOMO-1 in neighboring molecules in the thin films, and this effect can well simulate the photoelectron spectrum of frontier orbitals.　In contrast, the PAD of a well-ordered picene, which does not show a mixed orbital transport, revealed the distinct PAD pattern between HOMO and HOMO-1 due to the distinct shape of the wavefunctions. Therefore, the mixed-orbital carrier transport in DPh-BTBT can be attributed to its frontier orbitals with similar shapes, in addition to their efficient overlap in the well-ordered film.

Photophysics and Structure of 2D Perovskite Films for Optoelectronics

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Abstract ID: 10397
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: 2D perovskites, film structure, optoelectronics, photophysics

Films of quasi-2D Ruddlesdon-Popper perovskites (2D-RPPs) are under intensive study as candidates for various optoelectronic devices, as they exhibit superior stability compared to their 3D counterparts. 2D-RPPs have the general formula $R_2A_{n-1}Pb_nI_{3n+1}$ where A are small ammonium cations, R are long chain alkyl or aromatic cations that act as spacer groups for ‘n’ octahedral layers of $[PbI_6]^{4-}$. The structure of 2D-RPP films thus consists of perovskite slabs of various thickness separated by 2 layers of organic R ligands. The dielectric and quantum confinement imposed by the R layers make RPPs behave like quantum wells, with the bandgap tuned by altering the ‘n’ values. We report here on the application of spectroscopic and structural characterization techniques to (i) elucidate the role of the additive methyl ammonium chloride (MACl) in improving the efficiency of 2D perovskite solar cells, (ii) show how the complex microstructure of 2D-RPP films at various spatial scales affects the photophysical properties of the materials. The implications of the results for improving 2D perovskite device performance will be discussed.

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Polarized and Directional Electroluminescence from Organic Light-Emitting Devices by Using a Bifunctional Meta-Electrode

by Jing Feng | Shirong Wang | Yan-Gang Bi | State Key Laboratory on Integrated Optoelectronics, College of Electronic Science and Engineering, Jilin University | State Key Laboratory on Integrated Optoelectronics, College of Electronic Science and Engineering, Jilin University | State Key Laboratory on Integrated Optoelectronics, College of Electronic Science and Engineering, Jilin University

Abstract ID: 10497
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: OLEDs, Purcell Effect, SPP, directional emission, polarized

With the rapid development of immersive visual technologies and optical communication, there is a rapid surge in the demand for polarization and directional beam shaping of the light emission from the OLEDs. Existing implementation methods based on free space bulk optical elements suffer from significant power loss, limiting their practical applications. A bifunctional meta-electrode has been proposed by integrating a metasurface consisting of Ag periodic corrugations onto ITO anode to simultaneously realize the functions of charge carrier injection and photon management in OLEDs. We demonstrated highly polarized and directional light emission while maintaining a high device efficiency using the proposed meta-electrode. The electroluminescence with a polarization extinction ratio of 5 was achieved by judiciously engineering the polarization-dependent Purcell factor of the resonant cavity constructed by the meta-electrode. Meanwhile, the directional light emission with a divergence angle of 10° was also obtained by the efficient out-coupling of surface plasmon-polariton mode. The light beam can be tuned to normal to the surface of the OLEDs by using the corrugation period of 310 nm and can be collimated in two directions by using 2D nanopillars. Our results demonstrated that the proposed bifunctional meta-electrodes allowed for the realization the OLEDs with the tailorable directionality and polarization, and as well as maintaining high efficiency, promoting their broad applications in optical imaging, optical communication, immersive visual technologies, and many more.

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Precise and Scalable Synthesis of Conjugated Polymers

by Hui Huang | University of Chinese Academy of Sciences

Abstract ID: 10499
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: conjugated polymers, precise and scalable synthesis, structural defects, structure-property relationship

Conjugate polymers (CPs), especially the alternating CPs, have attracted much attention since they have applications in many fields, including energy, information, and biology. Currently, the synthesis of alternating CPs mainly depends on the transition metal-catalyzed cross coupling reactions. Due to the homocoupling side reactions, there are intrinsic structural defects in the backbones of the CPs, resulting in detrimental electronic properties, large batch-to-batch variation, and unclear structure-property relationship. Thus, it is important to develop new methods for precise and scalable synthesis of CPs.

In this talk, we will report several novel synthetic methods for precision synthesis of CPs including an original C-S bond activation based polymerization (CASP) method. We will discuss the catalytic systems, the structural defects and the catalytic mechanisms. Also, we will present the prospects and directions of this field.

Preparation of high-quality perovskite thin films and efficient fully printed carbon-based mesoscopic perovskite solar cells

by Prof. Jian Zhang | Guilin University of Electronic Technology

Abstract ID: 10467
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Perovskite thin film; Carbon-based perovskite solar cell; Interface regulation; Mesoporous structure

Carbon-based mesoporous perovskite solar cells (C-MPSCs) prepared based on a prefabricated three-layer mesoporous films (mesoporous TiO_2/mesoporous ZrO_2/porous Carbon) by fully printed technology have shown promising application prospects due to their excellent stability and convenient large-area preparation process. However, the power conversion efficiency (PCE) of C-MPSCs is restricted by the imbalance of carrier transport at the interface between the perovskite film and charge transport layer, as well as the difficulty in controlling the crystal quality of the perovskite film in the three-layer mesoporous films. In response to the key scientific issues mentioned above, we applied organic amine molecules to post-treat the perovskite films/Carbon interface. By in-situ room temperature reaction between organic amine molecules and FA^+ at the interface, large-sized organic cations were formed, and an embedded 2D/3D perovskite heterojunction was constructed, thereby optimizing the interface energy level arrangement, improving the interface hole extraction. Finally, C-MPSCs with PCE exceeding 20% were prepared, and the devices exhibited good stability. Furthermore, in response to the demand for low-cost preparation of high-quality perovskite films for large-area C-MPSCs modules, we have developed a low-boiling point mixed solvent based on 2-ME/NMP, which realized the preparation of high-quality perovskite films with high repeatability under annealing free conditions, and prepared C-MPSCs with PCE exceeding 18.5%.

Printing Organic and Perovskite Solar Cells and their Modules

by Junliang Yang | Hengyue Li | Erming Feng | Jianhui Chang | Central South University | Central South University | Central South University | Central South University

Abstract ID: 10098
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: organci solar cells; perovskite solar cells; modules; printing; doctor blading

Organic solar cells (OSCs) and perovskite solar cells (PSCs) have been considered as promise and competitive candidates for the next generation photovoltaics owing to their unique photovoltaic properties and a remarkable breakthrough in efficiency. In our group, recent efforts have been devoted to the fabrication of efficient and stable OSCs and PSCs via printing process. Through the optimization of printing parameters and the modulation of the interface layer and the active thin film, we achieved highly efficient OSCs with the power conversion efficiencies (PCEs) of over 18 %, which is comparable with spin-coated OSCs. Meanwhile, the OSC mini-modules (illumination area of 26.75 cm^2) with the certified power conversion efficiencies (PCEs) of 13.56% and 14.34% based on PM6:Y6 and PM6:Y6:PCBM, respectively, were achieved as well. Furthermore, we recently achieved 16.10% efficiency OSC modules (an active area of 11.08 cm^2) and a certified 15.43% efficiency OSC modules (an aperture area of 11.30 cm^2) with as small as 80 μm interconnection width and impressive geometric fill factor (GFF) of 98% processed by nanosecond ultraviolet laser, one of the highest PCEs among the currently reported OSC modules. On the other hand, low-dimensional intermediate phase induced by the methylamine chloride (MACl) additive could effectively regulate the crystallization of perovskite, resulting in a PCE of 23.14% and 21.20% for 0.09 cm^2 and 1.03 cm^2 PSCs, respectively, fabricated via two-step sequential doctor-blading process. An interface material 2-(N-Morpholino)ethanesulfonic acid potassium salt (MESK) is incorporated as the bridging buried interface layer enable 24.67%-efficiency doctor-bladed PSCs in ambient condition, and the mini-modules with an active area of 11.35 cm^2 exhibit a typical PCE of 19.45%. These results indicate that efficient and stable OSCs and PSCs, as well as their modules, could be achieved via the fabrication of printing techniques.

Progress in Organic Optoelectronic Films by means of Molecular and Nanoscale design

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Abstract ID: 10550
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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Organic semiconductors, devices, films, nanostructures, optoelectronics

Films are the key component of organic devices with various functionalities. In comparison to the inorganic films with the high energy-consumptive procedures and expensive equipment as well as the severe vacuum condition, organic films exhibit completely different preparation condition, such as the printing and roll-to-roll processes, and film features, such as large-area, light, flexibility as well as transparent and so on. In the context, we reported the flexible electronic films from the various nanostructures, including the conductive films of rGOs[1-3], the semiconducting films of emitters[4-6], as well as the dielectric films with the nanoporous or nanocolumn structures[7]. Especially, organic nanocrystalline films have been obtained by the step-by-step methods starting from the molecular design, followed by the organic synthesis and molecular assembly with the surfactant-assisted reprecipitation. The nanofilms offer state-of-the-art models to uncover the deep relationship between hierarchical structures and properties/ performance. Furthermore, meso-scale order films are the key components of not only optical materials but also various meta-materials. Organic polynanomers[8-11] have been successfully designed to give the flexible films with the excellent one-dimensional photonic crystals that are different from the liquid crystals that is not only used to the display but also multifunctional optical materials and elastic materials.

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Quinoid-Type Near-Infrared Organic Optoelectronic Materials and Their Functional Devices

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Abstract ID: 10358
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: near-infrared, organic optoelectronic materials, organic photodetectors, organic solar cells, performance

Photoelectric effect is an important cornerstone of modern science and technology and an important symbol of human civilization. Photovoltaic technology, which converts solar light energy into electric energy, is becoming more and more important under the background of national dual carbon strategy, and photodetection technology, which converts optical signals into electrical signals, has become an important part of modern information technology. Photoelectric conversion devices based on organic optoelectronic materials not only have the advantages of light weight, thinness, high flexibilty, and large-area processability, but also become increasingly prominent in future applications. Compared with monocrystal silicon technology, how to play its unique advantages of organic photovoltaic technology is the focus of attention in the field. Different from the characteristics of no selection and weak absorption under the band gap of silicon semiconductor materials, organic semiconductors have intrinsic strong structured absorption, which creates new opportunities for the research field of (semi) transparent solar cells and has irreplaceable advantages in the integrated application of photovoltaic buildings. Traditional near-infrared light detection technology is mainly based on inorganic semiconductors (such as InGaAs, GaAs alloys), which often needs to be used at low temperatures in order to improve the sensitivity. The development of near-infrared light detection technology has brought new solutions. The bulk heterojunction organic photovoltaic devices and photodetectors not only have similarities in operating principles, but also have differences in performance evaluation. The core of their performance depends on near-infrared organic optoelectronic materials and the optimized construction of devices based on near-infrared materials. Therefore, the development of high-performance near-infrared optoelectronic materials has become a common challenge for these two types of photoelectric conversion technologies. This report will introduce our important progress in the research of near-infrared organic optoelectronic materials and high-performance functional devices.

Realizing efficient blue and deep-blue delayed fluorescence materials with record-beating electroluminescence efficiencies of 43.4%

by Yan Fu, Hao Liu, Ben Zhong Tang, Zujin Zhao | State Key Laboratory of Luminescent Materials and Devices, Guangdong Provincial Key Laboratory of Luminescence from Molecular Aggregates, South China University of Technology, Guangzhou 510640, China.

Abstract ID: 10453
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: fine-tuned charge transfer strength, hyperfluorescence, thermally activated delayed fluorescence, ultrahigh-efficiency blue organic light-emitting diode

As promising luminescent materials for organic light-emitting diodes (OLEDs), thermally activated delayed fluorescence materials are booming vigorously in recent years, but robust blue ones still remain challenging. Herein, we report three highly efficient blue and deep-blue delayed fluorescence materials comprised of a weak electron acceptor chromeno[3,2-c]carbazol-8(5H)-one with a rigid polycyclic structure and a weak electron donor spiro[acridine-9,9’xanthene]. They hold distinguished merits of excellent photoluminescence quantum yields (99%), ultrahigh horizontal transition dipole ratios (93.6%), and fast radiative transition and reverse intersystem crossing, which furnish superb blue and deep-blue electroluminescence with Commission Internationale de I’Eclairage coordinates (CIEx,y) of (0.14, 0.18) and (0.14, 0.15) and record-beating external quantum efficiencies (ηexts) of 43.4% and 41.3%, respectively. Their efficiency roll-offs are successfully reduced by suppressing triplet-triplet and singlet-singlet annihilations. Moreover, high-performance deep-blue and green hyperfluorescence OLEDs are achieved by utilizing these materialsassensitizers for multi-resonance delayed fluorescence dopants, providing state-of-the-art ηexts of 32.5% (CIEx,y = 0.14, 0.10) and 37.6% (CIEx,y = 0.32, 0.64), respectively, as well as greatly advanced operational lifetimes. These splendid results can surely inspire the development of blue and deep-blue luminescent materials and devices.

Realizing Highly Stable Perovskite Quantum Dots for Opto-Electronic Applications

by Chang-Lyoul Lee | Gwangju Institute of Science and Technology (GIST)

Abstract ID: 10417
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Perovskite, Quantum Dots, Stability

Perovskite quantum dots (QDs) have attracted much attention as light-emitting materials for next-generation displays. Despite their outstanding properties, poor structural stability is an obstacle to the commercialization of perovskite QDs, which must be addressed. High structural stability can be achieved by introducing (1) UV cross-linking ligands, (2) core-shell structures, and (3) alkali metal doping. These methods minimized ligand dissociation and defect formation, resulting in improved structural stability.

Recent Progress in Organic Photovoltaic Materials

by Yingping Zou | Jun Yuan | Central South University | Central South University

Abstract ID: 10480
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: high electron mobility;energy disorder;quasi-macromolecules;highly efficient;acceptor

We proposed the design strategy of A-DA'D-A type molecules and synthesized a series of NIR small molecular acceptors (SMAs) with high electron mobility(BZIC, Y6, Y11, Y18,etc.) and decreased energy disorder. Also high performance star molecule Y6 was developed，promoting the rapid progress of photovoltaic efficiency. Recently we further provided the new strategy of A-π-A type “quasi-macromolecules” acceptor, achieving highly efficient and stable OSCs; Meanwhile, based on pentacyclic fused ring backbone, by altering the positions of oxygen, my group developed highly efficient, low cost NIR acceptors.

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Reducing the non-radiative charge recombination for high-performance organic solar cells

by Lijian Zuo | Zhejiang University

Abstract ID: 10314
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: non-radiative charge recombination, organic photovoltaics

Organic solar cells (OSCs) show promise as the next-generation renewable energy source for sustainability and carbon neutrality of the world, due to their merits of low-cost, good flexibility, light- weight, etc. The recent years have witnessed significant progress in OSCs, which shows a record efficiency over 20%. Nevertheless, further improving the device performance is still in need, and currently, the severe non-radiative charge recombination becomes the most important obstacle for further improving the device performance of OSCs. To resolve this issue, we identify that a third component with suitable physical and optoelectronic properties can significantly reduce the non-radiative charge recombination via suppressing the electron-vibration coupling, which we term it as the “dilution effect”.[1] Following this, we have developed more diverse and efficient third compoents and successive make breakthroughs in the world-record certified efficiency, which has greatly stimulated the progress of OSCs.

Remarkably Improved Photovoltaic Performance and Stability of Perovskite Solar Cells by Adoption of n-Type Cathode Interlayers

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Cathode interlayer, Perovskite solar cells, ion capture

Recently, inverted perovskite solar cells (PSCs) have witnessed significant advancements; low-temperature fabrication, enhanced device stability without doping, reduced hysteresis, and prospects for commercialization. However, despite these advantages, inverted PSCs still face challenges in achieving the power conversion efficiency (PCE) and stability comparable to their conventional counterparts. In particular, the PCE of inverted PSCs could be limited, which results from the unbalanced matching of energy levels between the electron transporting layer (ETL) and metal cathode. Therefore, extensive research efforts have been directed towards the integration of the cathode interlayer (CIL). In addition, silver (Ag) is a commonly used cathode material in inverted PSCs, and long-term stability of inverted PSCs is hampered by electrode corrosion. This degradation is mainly caused by the oxidation of Ag induced by its reaction with the iodide migrating from the photoactive perovskite layer. Furthermore, the Ag electrode can be thermally decomposed and moved into the perovskite layer, degrading the device's performance. Few strategies have been explored for physically blocking the perovskite layer and electrode to improve the stability of PSCs, however, the effects are very limited.

In this study, we present the development of NDI and PDI-based CILs aiming to enhance the photovoltaic performance and stability of inverted PSCs. By incorporating NDI and PDI-based CILs between the C_{60} electron transport layer (ETL) and the Ag cathode, we achieved high **power conversion efficiency (PCE) more than 23% together with remarkably high stability to maintain ~80% of the initial PCE over 1500 h at 85 °C (in N_2 without encapsulation) and over 500 h under 1-sun illumination** at room temperature and 25% relative humidity (RH) with encapsulation. We investigated the role and effects of the NDI and PDI-based CILs on device performance and stability were investigated in detail.

Reusable film-based fluorescent platform for sarin substitute and ammonia visual detection with an instantaneously-response

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Fluorescent probe, Fluoresent film, Sarin

Given the severe toxicity of Sarin and the hazardous implications of ammonia, efficient fluorescence detection of them is essential to reduce potential casualties. Till now, several probes have been developed for the detection of individual Sarin and ammonia, there is a demand for consecutive multiple-analyte detection. However, existing strategies of consecutive detection often rely on the replacement of two analytes, such as secondary coordination, typically in a liquid state and cannot be reused.

In view of the above, a novel small organic fluorescent molecule, DMATAZ, composed of a donor (D)-acceptor (A)-donor (D) structure based on 4H-1, 2, 4-triazole (TAZ), has been synthesized and applied as film-based probes for the detection of diethylchlorophosphate (DCP, a Sarin substitute), and ammonia vapor. Upon exposure to DCP, TAZ was attacked and subsequently protonated, along with a fluorescence color change from blue to green due to the enhancement of the intramolecular charge transfer (ICT) effect. The protonated probe was then used to detect ammonia vapor and finally generated the origin functional group of TAZ, manifesting an inverse fluorescence color change. More impressively, the probe displays instantaneously responses toward both DCP and ammonia vapors and the limit of detection (LOD) is as low as 1.4 ppb and 26 ppb, below the toxicity threshold limit value of 7 ppb and 25 ppm. The reusability of DMATAZ has also been validated through 10 sequential cycles. Further, visual testing filter paper-constructed strips based on DMATAZ have been fabricated to realize real-time, on-site, highly sensitive and recyclable monitor of DCP and ammonia vapors.

Revealing Design Rules for Improving The Photostability of Non-Fullerene Acceptors from Molecular to Aggregation Level

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: exciton dynamics, molecular aggregation, non-fullerene acceptors, or-ganic solar cells, photostability

With the rapid increase in power conversion efficiency of organic photovoltaics due to the development of non-fullerene acceptors (NFAs), prolonging the operational lifetime of devices becomes one of the critical prerequisites for commercial application. In this work, the degradation pathways of a wide range of state-of-the-art NFA molecules via multiple spectroscopic techniques combined with density functional theory and molecular dynamics simulation are revealed. The structural confinement and molecular ordering are responsible for molecular conformational stability under illumination. More importantly, a very general trend is revealed that the origin of increased nonradiative decay under illumination is predominately in the aggregated states with strong intermolecular interactions while the intramolecular exciton dynamics are stable. The increased nonradiative decay correlates with reduced exciton diffusion length. This work provides vital information toward the design of intrinsically photo-stable NFAs at the molecular level and the importance of aggregation control toward long-term stable organic solar cells.

Revealing the role of donor/acceptor interfaces in nonfullerene-acceptor based organic solar cells: charge separation versus recombination

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: organic solar cells; donor/acceptor interfaces; charge separation; radiative and nonradiative charge recombination

Organic solar cells (OSCs) based on nonfullerene acceptors (NFAs) have achieved rapid development, while the role of donor/acceptor (D/A) interfaces in NFA based heterosystems has not been fully addressed. Here, we clarify that the photoinduced spontaneous charge separation efficiency in typical NFA heterosystems can reach up to 67%, and the charge separation efficiency contributed by the D/A interface is only 25%. The more important role of D/A interfaces is reducing the charge recombination rate, especially optimizing the competition between radiative and nonradiative charge recombination, thus reducing the nonradiative voltage loss. Systematical simulations demonstrate that there exists an optimal interfacial distance for a fixed energy offset, at which the D/A interface can reduce the nonradiative voltage loss by a maximum value of 0.12 V. Hence, we propose that optimizing the interfacial distance combined with the actual interfacial energy offset of a given heterosystem is important to develop its best photovoltaic performance.

Self-healing Flexible Perovskite Solar Cells

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Flexibility, Perovskite Solar Cells, Self-healing

Flexible perovskite solar cells (FPSCs) stand as pivotal power sources, boasting high efficiency and seamless integration into various applications such as building windows and portable electronics. Despite their promise, the transition of FPSCs from laboratory research to commercial viability faces substantial hurdles, particularly concerning device stability and reliability. This presentation addresses these challenges, focusing on innovative approaches to enhance FPSC stability and performance. We introduce host-guest interaction-based ternary multifunctional polymers within 2D/3D heterostructures, and a dynamic "ligament" comprising supramolecular PDMS polypropylene urethane (DSSP-PPU) to facilitate perovskite grain boundaries, thereby improving the stability of FPSC devices. Additionally, we augment the stability and self-repair capabilities of FPSCs by incorporating a self-repairing nitrogen-oxygen radical dopant (DT-TEMPO) into the Spiro-OMeTAD. Our efforts yield promising results, with FPSCs achieving peak efficiencies of 25.67% on rigid substrates, 21.23% on rigid mini-modules, and 23.00% on flexible substrates. Furthermore, these flexible perovskite solar cells demonstrate remarkable self-healing efficiency, retaining nearly 95% of their initial efficiency even after 20,000 bending cycles. Through these advancements, we pave the way for the practical realization of FPSCs in diverse real-world applications.

Stabilizing interfaces with ordered polymer layers in planner- and bulk-heterojunction organic solar cells

by Yujie Xu | Xiaoyan Du | State Key Laboratory of Crystal Materials, School of Physics, Shandong University | State Key Laboratory of Crystal Materials, School of Physics, Shandong University

Abstract ID: 10046
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: crystallinity, interface, microstructure, organic solar cells, stability

With the soaring efficiency of single junction organic solar cells (OSCs), their commercialization process faces long-term device stability challenges. The complexity of the microstructure of the active layer and device structure makes mechanism research difficult. We have successfully constructed a planar heterojunction active layer, gained a deeper understanding of the interaction between the active layer and the interface, and revealed the mechanism of OSCs degradation under aging conditions. By precisely controlling the microstructure of the photoactive layer, it was found that the interaction between the hole transport layer and the polymer donor under illumination is the main degradation pathway, while the loss of fill factor under thermal stress comes from the mutual diffusion at the donor-acceptor interface. By increasing the crystallinity of polymer donors, these two degradation pathways can be effectively suppressed. In summary, we provide a new direction for the stability research of OSCs by precisely controlling their microstructure and optimizing their morphology. This study not only enhances our understanding of the degradation mechanism of OSCs, but also provides strong support for future device optimization and stability enhancement.

Studies on Quantum Quench Dynamics in Metallic Carbon Nanotubes

by Lei Shan | Hunan University

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: Quantum Quench Dynamics; low-dimensional carbon-based devices; Bosonization

Due to their unique structural advantages and excellent electrical properties, low-dimensional carbon-based devices play a significant role in the development of new electronic devices in the "post-Moore's Law" era. This has led to extensive in-depth research on device physics. Currently, theoretical research on low-dimensional carbon-based devices primarily focuses on simplified models, such as Luttinger liquid. However, research on experimentally preparable low-dimensional carbon-based devices, like carbon nanotubes, remains relatively scarce. The main bottleneck lies in the lack of efficient methods to address the complex electron-electron interactions in carbon nanotubes. We have developed a hybrid method that combines Bosonization and diagrammatic techniques. This method can accurately calculate the impact of electron interactions in carbon nanotubes on the photoelectric performance of the system.

Surface potential control by using polar small molecules with intermolecular hydrogen bonds

by Taiyo Inoue | Masahiro Ohara | Hisao Ishii | Chiba University | Chiba University | Chiba University

Abstract ID: 10398
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: effective work function, rotary kelvin probe, spontaneous orientation polarization

Electric polarization of organic layers is an important factor to control potential profile in organic films and interfaces; polarization at interface can induce interface dipole layer to modify the carrier injection properties, while the orientation polarization of polar molecules in the whole film can induce a huge potential difference across the film, called giant surface potential (GSP). GSP has been reported to have a significant impact on the performance of organic devices. Thus, the control of orientation polarization of polar organic molecules is a key technique to improve the performance of organic electronic devices.

In general, when molecules with permanent dipole moment (PDM) are aggregated, each PDM tends to have anti-parallel configuration because of dipole-dipole interaction. The introduction of other intermolecular interaction is one solution to overcome this effect.

In this study, we focus on hydrogen-bonding to overcome dipole-dipole interaction. The molecules that we investigated are nucleobases and related molecules which can aggregate through hydrogen bonding. The surface potentials of their films were measured by rotary Kelvin probe, a technique unique to our laboratory that enables simultaneous observation during film deposition.

We observed that the nucleobase guanine generates positive (25 mV/nm) and Adenine negative (-27 mV/nm) GSP, suggesting the possibility of polarity control of GSP by selecting molecular structure. In contrast, squaric acid does not show any GSP feature, but more than 1 eV vacuum level shift was observed at ITO interface, indicating the increase of the effective work function. Thus, the insertion of squaric acid is expected to improve the hole injection property at organic/ITO interface. The above results show the promise of molecules with hydrogen-bonding unit as electronic materials.

Tailored Molecular Orientation Polarization Control in Organic Amorphous Films through Intermittent Deposition Method

by Masahiro Ohara | Taiyo Inoue | Hisao Ishii | Chiba University | Chiba University | Chiba University

Abstract ID: 10430
: ThinFilms2024
Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: molecular orientation, organic light-emitting diode, rotary Kelvin probe, spontaneous orientation polarization

Organic optoelectronic devices rely on molecular orientation to achieve optimum performance. Asymmetric molecules are employed to form pinhole-free amorphous thin films. Asymmetric molecules often have a permanent dipole moment, which causes spontaneous orientation polarization (SOP) in the film thickness direction due to the anisotropic molecular orientation[1,2]. It is crucial for carrier injection, transport, and light extraction properties of the device. Molecular orientation is usually controlled by adjusting the substrate temperature and deposition rate.

The physical vapor deposition process involves molecular adsorption, diffusion, and collision, leading to film formation. Adjusting substrate temperature and deposition rate influences the diffusion time of molecules on the substrate surface, affecting their arrangement. However, the timescales controlled by these parameters are limited, necessitating alternative methods for achieving desired molecular orientations.

This study explores the use of intermittent deposition intervals as a novel technique for SOP control. By periodically opening and closing the deposition shutter, the relaxation time of molecules on the substrate surface can be modified, allowing for tailored molecular orientation. The impact of this approach on organic semiconductor films, specifically tris(8-hydroxyquinolinato)aluminum (Alq3) and 1,3,5-tris(1-phenyl-1H-benzimidazol-2-yl)benzene (TPBi), were investigated.

Real-time surface potential measurements using a rotary Kelvin probe[3,4] revealed orientation relaxation occurring within seconds after shutter closure. Repeating intermittent deposition could alter the magnitude and even the direction of SOP. Notably, the polarization direction in Alq3 films was successfully switched, creating potential valleys in a single-component film. This technique offers the potential for arbitrary modification of potential profiles in films, enabling precise tuning of conduction properties and the realization of specialized device functionalities.

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The correlation between reduction potentials by cyclic voltammetry and electron affinities by low-energy inverse photoelectron spectroscopy

by Mihiro Kubo | Hiroyuki Yoshida | Chiba University | Chiba University

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: cyclic voltammetery, electron affinity, low-energy inverse photoelectron spectroscopy, reduction potential

The electron affinity (A) of organic semiconductors represents the electron conduction level. In many studies, A is estimated from the reduction potential (E_{red}) measured in solution by cyclic voltammetry (CV). To convert E_{red} to A, a linear relationship, $A=\alpha*E_{\mathrm{red}}+\beta$, with the values of $\alpha=1$ and $\beta=4.8$ eV (the energy of ferrocene) is often used. In contrast, we can directly measure A in solid by low-energy inverse photoelectron spectroscopy (LEIPS) with a precision of 0.1 eV. In this study, we re-examined the correlation using A measured by LEIPS. We considered prototypical semiconductors such as pentacene, OLED molecules, and organic solar cell molecules as fullerene derivatives and non-fullerene acceptors (NFAs). Based on the precisely determined A values, we propose improved conversion parameters α and β to predict A in solid from E_{red} measured in solution.

The effect of weak density-of-states above HOMO/Valence band onset on electric properties of organic and inorganic semiconductors

by Hisao Ishii | Ryotaro Nakazawa | Kohei Shimizu | Chiba University | Chiba University | Chiba University

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: carrier density, carrier injection, density-of-states, photoemission spectroscopy, semiconductor

It is widely accepted that the HOMO (or LUMO) onset of the organic semiconductors play an important role in electric processes such as carrier injection and transport. The same holds for inorganic semiconductors. Such an onset position has been investigated by using UV photoelectron spectroscopy (UPS) for various materials, in which the linear part of the HOMO peak in UPS spectrum is extrapolated to the background level to determine the onset. For organic semiconductors, the distributions of the density-of-states (DOS) of the HOMO and LUMO are widely assumed to be Gaussian functions. The onset position of the Gaussian (often corresponds to the position shifted by 2σ from the peak) has been also used to estimate HOMO onset. In this case, the DOS at the onset is roughly one order of magnitude smaller than that of the HOMO peak. But the probability of generating holes is extremely low because of the large energy separation (often 0.5 to more than 1 eV depending on materials) from the Fermi level of the electrode (the Boltzmann factor for 500 meV is $<10^{-10}$ at 300 K). In contrast, the probability becomes very large for shallower tail states in the HOMO–LUMO gap with extremely low DOS. Owing to these reasons, the shallower states with lower DOS should also be taken into account.

In this study, we have observed the weak DOS of α-NPD films by using high-sensitivity UV photoemission spectroscopy (HS-UPS), and tried to simulate the hole injection properties at α-NPD/HAT-CN/ITO interface. Also, the possible hole density in α-NPD film was also estimated to discuss hole transport. Then we would like to demonstrate the DOS at shallower than HOMO onset is critical to explain the practical electric properties. The results for inorganic p-type semiconductors will be also reported.

Ultrafast charge carrier dynamics in graphite and metal/semiconductor nanostructures revealed by femtosecond diffuse reflectance spectroscopy

by Akihiro Furube | Tokushima University

Abstract ID: 10481
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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: , nanoparticle, optical switching, photocatalyst, plasmon, ultrafast spectroscopy

Nanostructures composed of materials with excellent optical absorption, charge mobility, surface reactivity, and stability can offer important applications such as ultrafast optical switching, photodetection, solar cells, photocatalysts, photothermal conversion, and more. In this study, laser-ablated graphite nanoparticles with ultrafast optical responses and a silver nanowire (AgNW)/TiO2 deposition film with high photocatalytic performance were prepared to investigate their primary processes occurring on the femto- and pico-second time scales. Femtosecond diffuse reflectance spectroscopy was utilized to observe transient absorption of these opaque samples.

Transient absorption spectroscopy confirmed the ultrafast excitation of ablated graphite with the carrier relaxation occurred around 300 fs. A reference reduced graphene oxide (rGO) powder showed TA intensity about 6.7%, while the graphite sample showed 3.5%. Although rGO shows higher absorption intensity than the graphite samples, much cheaper graphite should be useful for the future application of optical switching.

AgNW/TiO_2 samples were prepared using a commercial TiO2 spray. The surface structure of the samples was also observed by SEM image analysis for the prepared samples to confirm that the TiO_2 particles were sufficiently attached to the AgNW surface. In order to evaluate the photocatalytic activity, a decolorization experiment of methylene blue was conducted, and it was confirmed that the AgNW/TiO_2 sample prepared in this study decomposes methylene blue more efficiently than a single sample. To confirm that the photocatalytic reaction is caused by the interaction between AgNWs and TiO_2, the electron transfer dynamics between AgNWs and TiO_2 was observed under the excitation of the plasmon band of AgNWs using transient absorption spectroscopy.

Ultrafast Spin Manipulation in Organic and Hybrid Semiconductors*

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: chiral-induced spin selectivity (CISS) effect, singlet fission, spintronics, triplet fission

Spintronics has experienced rapid development in the past few decades, and spin devices based on new materials and principles have emerged one after another, revolutionizing the methods and means of spin state control. Exploring new principles of information devices based on spin as an information carrier has become a significant development trend. Recently, we have conducted a series of studies on spin manipulation and control, spin lifetime, and other vital issues using femtosecond transient spectroscopy and its magnetic field control. We observed a giant Rashba effect in two-dimensional perovskite through optical methods. We successfully realized a perovskite spin optoelectronic device that does not require external magnetic fields or ferromagnetic contacts at room temperature using the chiral-induced spin selectivity (CISS) effect. We also observed a giant magneto photoluminescence (MPL) by manipulating the balance of singlet and triplet states in organic microcrystals.

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Well-crystallized epitaxial thin films of molecular semiconductors on organic semiconductor single crystals (II)

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: heteroepitaxy, organic semiconductor, single-crystal

Organic optoelectronic devices are generally driven by electronic processes at heterojunctions which are bi-molecular contacts of “p-type” (donor) and “n-type” (acceptor) molecular semiconductors. Although standard organic optoelectronic devices are made of amorphous or polycrystalline thin films of molecules, well-crystallization of the semiconductor media, e.g. utilization of single-crystalline materials, has been regarded as one promising route for pursuing competitive performance of the organic devices to their inorganic counterparts because charge carriers are potentially liberated from single molecular ions to delocalized electrons and holes thanks to the intermolecular electronic band dispersion enabled in highly-ordered molecular arrangements [1].

Epitaxy is an established technology for constructing well-crystallized semiconductor materials. Our group has studied epitaxial growth of semiconducting molecules on organic molecular single crystal surfaces [2], which we introduced in a previous edition of this conference (ThinFilms2018). In this contribution, we report our recent achievements on epitaxial heterojunctions between prototypical molecular semiconductors (e.g., perfluorophthalocyanine copper (C32CuF16N8) on the single-crystal phthalocyanine copper (C32CuH16N8) [3] and C60 on the single-crystal dinaphtho[2,3-b:2’,3’-f]thieno[3,2-b]thiophene (C22H12S2) [4]) and also on the “quasi-homoepitaxial” junction of very high crystallinity between bis(trifluoromethyl)dimethylrubrene (C46H30F6) and the single-crystal rubrene (C42H28) [5].

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π-π stacking modulation via polymer adsorption for elongated exciton diffusion in high-efficiency thick-film organic solar cells

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Symposium: 9. Organic Electronics and Photonics (OEP)
Keywords: exciton diffusion, intermolecular interaction, thick film organic solar cells

Despite the progress made in organic solar cells (OSCs) in recent years, their widespread commercial implementation remains challenging. One major obstacle is the limitation on the thickness of the active layer, which is currently confined to a narrow range of 80 nm to 120 nm for high-efficiency devices. Thin-film OSCs used in lab-scale experiments are not compatible with industrial production due to difficulties in achieving homogeneous and defect-free films. Therefore, developing efficient thick-film OSCs is crucial for successful industrial production. However, thick-film OSCs face challenges such as enhanced charge recombination and trap states, which hamper their overall device performance.

This study addresses the challenge of maintaining efficiency in thick-film organic solar cells (OSCs) for large-scale manufacturing. We have developed a novel polymer adsorption strategy that regulates molecular stacking within the active layer, leading to enhanced intermolecular interactions and improved electron wave function overlapping. This results in more ordered molecular alignment, extending exciton lifetime and diffusion length. By leveraging this approach, we achieved a reduction in trap states and an elongation in exciton diffusion length, resulting in a remarkable increase in power conversion efficiency (PCE) in thick-film OSCs. Our findings represent a critical advancement towards the successful transition of thick-film OSCs from laboratory research to industrial production.