PROGRAM

Frontiers Symposium of the Basic Research Center of Excellence for Energy & Information Polymer Materials

Series 2: Organic Optoelectronic Materials and Devices - Surfaces/Interfaces Physics and Chemistry

Symposium Schedule

Apr. 26 Morning	Venue: N308 lecture hall		
09:20-09:30	**Welcome Speech**		**Yuguang Ma**
Moderator: Liang Yao			
Time	Speaker	Affiliation	Title
09:30-10:10	Mats Falman	Linköping University	Organic semiconductor materials and interfaces
10:10-10:50	Junwu Chen	South China University of Technology	Morphological control of organic active layer in polymer solar cells
10:50-11:30	Qinye Bao	East China Normal University	Heterointerface energetics in perovskite solar cells
11:30-12:10	Xuhui Zhu	South China University of Technology	Phen-NaDPO: a multifunctional 1,10-phenanthroline derivative for optoelectronics
Lunch			
Apr. 26 Afternoon	**Venue: N308 lecture hall**		
Moderator: Xuhui Zhu			
Time	Speaker	Affiliation	Title
14:30-15:10	Xianjie Liu	Linköping University	Probe organic materials upon advanced electron/x-ray spectroscopies
15:10-15:50	Liang Yao	South China University of Technology	Organic π-conjugated materials for (photo-)electrocatalysis
15:50-16:00	**Coffee Break**		
16:00-16:20	Qilun Zhang	Linköping University	Industrial lignin based binary cathode interface layer in organic solar cells
16:20-16:40	Haoran Tang	South China University of Technology	Development of n-type conducting polymers and their carrier transport properties
16:40-17:00	Xiane Li	Linköping University	Mapping the energy level alignment at donor/acceptor interfaces in non-fullerene organic solar cells
17:00-17:20	Yanuo Zhu	South China University of Technology	Organic Ferromagnetic Semiconductors
17:20-17:30	**Concluding Speech**		**Mats Falman**

Speakers Introduction

1 Speaker

Mats Falman

Professor, Faculty of Science and Technology, Linköping University, Sweden, Director of the Organic Electronics Laboratory, Vice President of the Natural and Engineering Sciences Directorate of the Swedish Research Council, and Adjunct Professor, Wallenberg Wood Science Centre, Sweden. He was a member of the Board of Directors and the Science and Technology Committee of the National Synchrotron Radiation Laboratory.

Title: Organic semiconductor materials and interfaces

Abstract: Organic semiconductor materials can be used in a wide variety of technological applications such as energy conversion, light emission and sensing. In the corresponding devices, many key processes (e.g. charge injection from metallic electrodes, charge recombination into light or light conversion into charges, etc.) occur at interfaces and it thus is of great importance to understand and predict energy level alignment at both metal-organic and organic-organic interfaces. Here we will give an overview on energy level alignment at such interfaces and give examples of how photoelectron spectroscopy and various

synchrotron radiation-based techniques can shed light on device functionality in e.g. photovoltaics, transistors, thermoelectrics and spintronics.

2 Speaker

Junwu Chen

Prof. Junwu Chen received his B.S. degree in 1989 and Ph.D. degree in 1998. After postdoctoral research at Hong Kong University of Science & Technology, he held an associate professor in 2002 and a full professor in 2007 at South China University of Technology, Institute of Polymer Optoelectronic Materials and Devices, State Key Laboratory of Luminescent Materials and Devices. His research interests focus on synthesis of organic functional materials and their optoelectronic device applications.

Title: Morphological control of organic active layer in polymer solar cells

Abstract: Solvent additives have been employed to regulate bulk-heterojunction morphology of organic active layer for efficient organic solar cells (OSCs). With fullerene acceptor, Polymers PTB7 and PBT7-Th are two representative donors to construct high performing active layers that require the use of high boiling solvent additive 1,8-diiodooctane (DIO) to regulate the morphology. However,

due to high boiling point, DIO needs to be completely removed under vacuum drying, which leads to a more complicated process for the solution processing. We found that using some low boiling point solvent additives instead of DIO can significantly improve the morphology of the fullerene based active layers, achieving better efficiency for the thick-films. For example, PBT7-Th can achieve a maximum efficiency of over 10% at 230 nm. At the same time, using low boiling point additives has the characteristic of rapid removal, which can be removed together with the main solvent during spin coating without the vacuum process required by DIO. Recently, we have continued to propose a rapid removal strategy for solid additives in non-fullerene based active layer systems. By selecting low melting point solid additive, its in-situ removal can be achieved during the spin-coating process, resulting in device efficiency exceeding 19%.

We introduce siloxane-terminated side chains into polymer donors, polymer acceptors, small molecule donors, and small molecule acceptors to conduct side chain engineering research. High hole mobility polymer PFBT4T-C5Si-25% (Si25) exhibits 3D high mobility properties, with a hole mobility of 2.46 $cm^2/(V\ s)$ in OFET devices. Its pure and blended films can exhibit SCLC hole mobility of 10^{-2} $cm^2/(V\ s)$, making it particularly suitable for construct high-efficiency thick-film OSCs. The efficiency of the 420 nm thick Si25:$PC_{71}BM$ active layer can reach 11.09%. The active layer based on Si25 and non-fullerene acceptor Y14 shows an efficiency of 15.39% at 430 nm, and a thicker 600 nm active layer still remains an efficiency above 15%. Two characteristics have been found. Firstly, compared to

common alkyl, alkoxy, and alkylthio side chain substitutions, the introduction of siloxane-terminated side chains can endow photovoltaic materials with lower surface energy, resulting in changing of Flory-Huggins interaction parameter (χ_{DA}) between the donor and acceptor, providing a new chemical method to regulate BHJ phase separation and opening a space to improve the efficiency of OSCs. Secondly, the introduction of siloxane-terminated side chains can achieve device efficiency comparable to nitrogen glove boxes when processing active layers in high humidity air, which can avoid the significant decrease of efficiency of conventional active layers during processing in high humidity air. For example, in an air environment with 90% high relative humidity (RH), the active layer using siloxane-terminated side chains can achieve 18% efficiency, which is crucial for the industrial application of OSCs.

3 Speaker

Qinye Bao

Professor, School of Physics and Electronic Science, East China Normal University

Title: Heterointerface energetics in perovskite solar cells

Abstract: Organic-inorganic perovskite semiconductors have attracted tremendous attention owning to advantages of many exceptional optoelectronic properties such as high absorption coefficients, long carrier diffusion lengths, and adjustable band gaps, which enable them to be a promising photovoltaic material. Heterointerface energetics play a critical role in many key electronic processes of perovskite solar cells, e.g. charge injection/extraction, and recombination, significantly governing the final output efficiency and lifetime. In this talk, we will show our recent work on the electronic structures at perovskite heterointerface especially via photoelectron spectroscopy (UPS/IPES/XPS), which provide guidance for achieving high-performance perovskite solar cells with small energy loss.

4 Speaker

Xuhui Zhu

Professor, State Key Laboratory of Luminescent Materials and Devices, Institute of Polymer Optoelectronic Materials and Devices, South China University of Technology.

Title: Phen-NaDPO: a multifunctional 1,10-phenanthroline derivative for optoelectronics

Abstract: 3-[6-(diphenylphosphinyl) − 2-naphthalenyl] − 1,10-Phenanthroline (Phen-NaDPO, MW = 506.54) is a versatile cathode interlayer for efficiency and stability enhancement in optoelectronics. With respect to bathocuproine (BCP) and bathophenanthroline (BPhen), it possesses an enhanced glass transition temperature of 116 °C with a highest occupied molecular orbital (HOMO)/lowest unoccupied molecular orbital (LUMO) energy level of − 6.10/ − 2.74 eV. It is soluble both in weakly polar solvents e. g. toluene and strongly polar solvents, e. g., isopropanol. The X-ray structural analysis on a Phen-NaDPO single-crystal grown from solution shows that there are two neat molecules in the unit cell. In addition to efficient cathode modification, Phen-NaDPO and/or its isomer 5-[6-(diphenylphosphinyl)−2-naphthalenyl]−1,10-Phenanthroline find attractive applications in sensitizing the luminance of rare earth Eu (III) ion and as electron-generation layer in stacked OLEDs. The molecular structure and properties relationship shall be discussed.

5 Speaker

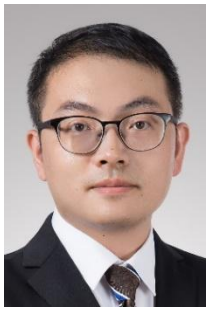
Xianjie Liu

Associate Professor, School of Science and Technology, Linköping University

Title: Probe organic materials upon advanced electron/x-ray spectroscopies

Abstract: The emergence of new organic materials not only enhance the performance of the corresponding organic electronic devices, but also bring novel science. Understanding the electronic properties of these organic materials is of vital importance for the materials development and applications, in which the application of the advanced x-ray/electron spectroscopies plays a crucial role in the development of this scientific topic. Here I will introduce various x-ray/electron spectroscopic methods to explore the state-of-the-art novel and high-performance organic materials upon their interface, valence/conduction electronic structure, and doping with the selection of materials from two-dimensional organic single crystal to pi-conjugated polymers. Finally, the novel feature of recently developed high-conductive n-type polymer PBFDO will be discussed.

6 Speaker



Liang Yao

Professor, School of Materials Science and Engineering, South China University of Technology

Title: Organic π-conjugated materials for (photo-)electrocatalysis

Abstract: Converting solar energy into chemical commodities (such as, hydrogen, hydrocarbons) via photoelectrochemical devices has become the topic of vital importance, since such a technique provides an efficient strategy for addressing solar energy intermittency problem and supplying feedstocks to the commodity chemicals industry on a global scale. Employing organic conjugated semiconductors in photoelectrochemical devices, including small molecules, linear polymers and covalent organic frameworks (COFs), is attracting an increasing interest in recent years, due to their tunable optoelectronic properties at the atomic level. So far, developing molecular designs and photoelectrode architectures toward achieving comparable performance and stability with inorganic counterparts remains as the major task of organic photoelectrodes. In this presentation, strategies for advancing the performance and operational stability of organic photoelectrodes will be discussed. Beyond that, latest research about CO_2 conversion with COF electrocatalysts will also be introduced.

7 Speaker

Qilun Zhang

Senior Research Engineer, Faculty of Science and Technology, Linköping University

Title: Industrial lignin based binary cathode interface layer in organic solar cells

Abstract: Herein, a binary cathode interface layer (CIL) strategy based on the industrial solvent fractionated LignoBoost Kraft lignin (KL) is adopted for fabrication of organic solar cells (OSCs).1 Lignin, with its phenolic and aliphatic hydroxyl functionalities acting as chemical handles, has potential as a material for binary systems composites, offering new insight to the interface challenges.2 The uniform-distributed multiple phenol enables KL to easily form bonds with commonly used CIL materials, i.e., bathocuproine (BCP) and PFN-Br, resulting in binary CILs with tunable work function (WF). The binary CILs work well in OSCs with large KL ratio compatibility, exhibiting equivalent or even higher efficiency to the traditional CILs in state of art OSCs.3 In addition, the combination of KL and BCP significantly enhanced OSC stability, owing to KL blocking the reaction between BCP and non-fullerene acceptors (NFAs). The lignin component is expected to act as hole- and exciton blocker, improve interface adhesion and passivate defects, which can be potentially used in perovskite solar cells (PSCs).

For instance, the PCBM/BCP bilayer is widely used at the heterointerface of PSCs with inverted architecture, possibly can be further optimized by the incorporation of KL in both sides. This work provides a simple and effective way to achieve highly efficient stable and sustainable OSCs and the potential application in PSCs.

8 Speaker

Haoran Tang

Postdoctor, South China University of Technology

Title: Development of n-type conducting polymers and their carrier transport properties

Abstract: Conducting polymers (CPs) with high conductivity and solution-processability have gained great advances since the pioneering work on doped polyacetylene. Various high-performance CPs have been realized, which enable the applications of multiple organic electronic devices. Nevertheless, most CPs exhibit hole-dominant (p-type) transport behaviour, while the development of n-type analogues lags far behind, typically limited by low doping efficiency and ambient instability. Through the structure modification and synthesis optimization, a solution-processed n-type conducting polymer with ultrahigh

conductivity (>2000 S/cm) was developed, bringing new insights into printed electrodes and organic circuits. Based on these newly developed n-type conjugated polymers, high performance OSCs, organic thermoelectric devices and organic electrochemical transistors were realized. We have also recently developed new building blocks that will further expand the range of n-type conducting polymers.

9 Speaker

Xiane Li

Postdoctor, Linköping University

Title: Mapping the energy level alignment at donor/acceptor interfaces in non-fullerene organic solar cells

Abstract: Energy level alignment (ELA) at donor (D) -acceptor (A) heterojunctions is an essential property that has a strong influence on the charge generation and recombination process in organic photovoltaic devices. However, the ELA at the D-A interfaces is largely underdetermined, resulting in debates on the fundamental operating mechanisms of high-efficiency non-fullerene organic solar cells. Here, we systematically investigate ELA and its depth-dependent variation of a range of donor/non-fullerene-acceptor interfaces by fabricating

and characterizing D-A quasi bilayers and planar bilayers. In contrast to previous assumptions, we observe significant vacuum level (VL) shifts from all the D-A interfaces, which result in reduced interfacial energetic offsets and increased charge transfer (CT) state energies. The VL shifts are demonstrated to be abrupt, extending over only 1 – 2 layers at the heterojunctions, and are attributed to interface dipoles induced by D-A electrostatic potential differences. The VL-shift-enhanced energy gap at the heterojunctions rationalizes high CT energies and high open-circuit voltages of corresponding organic solar cell devices. As such, our results reconcile the conflicting observations of large energy level offsets inferred from neat films and large CT energies of donor - non-fullerene-acceptor systems.

10 Speaker

Yanuo Zhu

Yanuo Zhu is now studying for a doctor's degree in State Key Laboratory of Luminescent Materials and Devices, South China University of Technology under the guidance of Prof. Yuguang Ma. The main research direction is organic ferromagnetic semiconductor materials and devices.

Title: Organic Ferromagnetic Semiconductors

Abstract: Due to the strong coulomb interaction between electrons and the coupling of electrons with orbits, spins, and other degrees of freedom, a series of novel phenomena, such as room temperature ferromagnetism, that are not found in the framework of single electrons, are generated in electron strongly correlated materials. These unknown physical states have profound physical connotations and broad application prospects and are the hot and challenging problems in the front of condensate physics. Magnetic semiconductors, which have both semiconductor and magnetic properties, are expected to solve the "post-Moore" problem. One of the 125 most challenging scientific questions published in the 125th-anniversary issue of Science: Can we make magnetic semiconductors at room temperature? Organic ferromagnetic semiconductor requires both semiconductor and magnetic characteristics, in which electrons have the property of delocalization. In contrast, the realization of magnetism requires electrons to have the property of solid correlation. Achieving the unity of the two in the same material is a critical scientific problem in the field of organic ferromagnetic semiconductors. This presentation presents recent advances in room-temperature ferromagnetic semiconductors with particular attention to structural regulation and strong intermolecular interactions from a chemical perspective. Perylene diimide aggregates containing high-density free radicals were prepared by ionization-induced reconfiguration strategy, which solved the problem of the weak correlation between molecules of free radicals and

promoted the formation of a long-range ordered arrangement of magnetic domains. The organic magnetic semiconductor at room temperature was realized for the first time with high saturation magnetization and high Curie temperature, showing excellent semiconductor properties. A magnetically controllable naphthalene diimide material system was developed. A "dispersion free radical bond model" was proposed based on the theoretical calculation to construct the strong spin interaction between free radicals and realize the organic magnetic semiconductor.