RGC Ref.: *N_HKBU202/16*
NSFC Ref. : *6161101026*
(please insert ref. above)

The Research Grants Council of Hong Kong
NSFC/RGC Joint Research Scheme
Joint Completion Report

(Please attach a copy of the completion report submitted to the NSFC by the Mainland researcher)

Part A: The Project and Investigator(s)

1. Project Title

Unraveling the fundamental mechanism of synergistic effect in ternary bulk-heterojunction blends for photovoltaic applications
有機光伏三元體相異質結構中的協同效應機制研究

2. Investigator(s) and Academic Department/Units Involved

	Hong Kong Team	Mainland Team
Name of Principal Investigator *(with title)*	Professor So Shu Kong (蘇樹江教授)	Professor Hao Xiaotao (郝曉濤教授)
Post	Professor	Professor
Unit / Department / Institution	Physics Department / HKBU (香港浸會大學)	Physics Department / Shandong University (SDU) (山東大學)
Contact Information	skso@hkbu.edu.hk	haoxt@sdu.edu.cn
Co-investigator(s) *(with title and institution)*		Associate Professor Gao Kun (高琨副教授) (SDU) Dr Zheng Fei (郑飞博士) Mr Bi Pengqing (毕鹏青) Mr Yang Xiaoyu (杨小雨) Ms Niu Mengsi (牛梦思) Mr Wang Yanbo (王彦博)

3. Project Duration

	Original	Revised	Date of RGC/ Institution Approval *(must be quoted*)
Project Start date	1 Jan 2017		
Project Completion date	31 Dec 2020		
Duration *(in month)*	48		
Deadline for Submission of Completion Report	5 Feb 2021		

Part B: The Completion Report

5. Project Objectives

5.1 Objectives as per original application

1. Identify suitable ternary bulk-heterojunction (BHJ) blends model systems for optoelectronic characterizations
2. Investigate potentially useful small molecules for enhancing hole conductivity in ternary blends
3. Explore thick film ternary BHJ blends with a suitable model ternary system

5.2 Revised Objectives

Date of approval from the RGC: _____

Reasons for the change: _____

_____

1.
2.
3. ....

6. Research Outcome

Major findings and research outcome

(maximum 1 page; please make reference to Part C where necessary)

We identified hole [1,2] and electron ternary compounds [3] and studied their beneficial roles in some benchmarked BHJ OPV cells. (**Objective (1)**).[1-3] In [1]-[3], we showed ternary components enhance hole/electron mobilities (2-3 times) and reduce electronic disorders. These observations are well correlated with improved fill factors (FFs) of the ternary BHJ cells. Our findings show small molecules [1] and polymers [2,3] can be used as a ternary component and improve electronic properties of binary BHJ in a ternary cell. From the concept and methodology established in Objective (1), we identified a hole conducting polymer PDTSTPD (**Objective (2)**) as a ternary compound to a binary BHJ of PCDTBT:PC71BM for room light harvesting.[2] A superior PCE exceeding 20% can be achieved under room light illumination, up from about 16% for a binary BHJ. The hole mobility of the ternary blend was enhanced by half order after addition of polymeric PDTSTPD due to its high hole mobility and compatible HOMO level with the PCDTBT. This work [2] has generated considerable attentions as it is the first reported literature for indoor OPV devices with PCE exceeding 20%. Moreover, it demonstrated that a ternary strategy can further improve some under-performed polymers. To realize a thick film BHJ cell (**Objective (3)**), we investigated a hole conducting small molecule DTS as a ternary component in some exemplary BHJ cells. We found that the FF plays the most important role. We then studied how the FF varies with the donor-to-acceptor (DA) weight ratio.[4] We introduced a new concept, known as the charge imbalance factor, and correlate this factor with the BHJ cell's FF. The best FF corresponds to a minimum imbalance factor. This concept was applied to explain the device FF dependence on BHJ cells in perylene diimide acceptors.[4] We also investigated the role of insulators on electron conduction in a BHJ containing polymeric N2200 as the electron transporter. We found that the substitution of N2200 by insulating polystyrene promotes electron transport, device performance and stability.[5]

Various BHJ systems were fabricated to study how morphology and phase distribution correlate with photophysical processes and device performance.[6-7] In [6], addition of $PC_{71}BM$ optimized the phase distribution in the vertical direction and promoted the extraction of free charge. Grazing-incidence wide-angle X-ray scattering (GIWAXS) indicated improved π-π stacking for host D/A in the ternary blend, which enhanced the charge mobility and suppressed the bimolecular recombination. Consequently, the PV devices with the ideal ternary morphology enjoyed the extraordinary performance. In [7], we found significant ternary mixed domains. Structural characterization methods combined with transient spectra showed improved crystallinity of donor in ternary BHJ blend, implying an additional channel for charge transfer and transport, leading to an improved excited state characteristic and PV performance. We also demonstrated enhanced energy transfer between the active materials in ternary compounds.[8-9] From [8], we reveal a large overlap between the emission of the third component and the absorptions of the host acceptor, which demonstrates Förster resonance energy transfer process in ternary blend, resulting in accelerated the ultrafast hole transfer process and improved the PCE and stability. In addition, we explored the effect of energy transfer on exciton dynamics on the ultrafast temporal scale in ternary blends and quantitatively studied the exciton diffusion length.[9] Through ultrafast spectroscopy, we found an enhanced energy transfer when fullerene acceptor serves as the third component in non-fullerene host systems. Therefore, the length for exciton diffusion is improved, indicating higher and more stable performance in ternary device compared to that of binary one. These results provided insights into BHJ morphology and energy transfer process in ternary BHJ blend and open a novel horizon for improving the efficiency of ternary photovoltaic devices.

References [1-10]: *Please see Part (C)*

Potential for further development of the research and the proposed course of action *(maximum half a page)*

With major advances in non-fullerene acceptors, particularly those emerging out of the development in new Y acceptors, new family of BHJ for ternary OPV cells can be further explored. We note that the Y acceptors have very small energetic disorder (even in a BHJ), which leads to devices with small FF. Thus, they should serve as good candidates for thick film BHJ cells. Suitable ternary compounds in these BHJs should give much better performed thick film BHJ cells for roll-to-roll printing.

7. The Layman's Summary

(describe in layman's language the nature, significance and value of the research project, in no more than 200 words)

An organic solar cell consists of a blend film to absorb solar energy and generate electricity. This collaborative project studied how such a solar cell can benefit from a ternary (3-compoent) blend film formulation consisting of a light-absorbing host polymer, an electron extracting acceptor, and a ternary component. The beneficial roles of ternary components were investigated in details, with the HK PI focusing on electrical characterization and the Mainland PI on the optical characterization. Through some exemplary model systems with thoroughly investigated experimental and models, we identified suitable ternary components that can enhance the electrical conductivities of blends, facilitate conversion of light energy, and improve their morphologies. Such knowledge leads to improvement in the power conversion efficiency of the solar cells, and allows new material and device strategies for fabricating thick film organic cells that are readily applicable for roll-to-roll manufacturing technology.

Part C: Research Output

8. Peer-reviewed journal publication(s) arising directly from this research project

(Please attach a copy of each publication and/or the letter of acceptance if not yet submitted in the previous progress report(s). All listed publications must acknowledge RGC's funding support by quoting the specific grant reference.)

The Latest Status of Publications				Author(s) ***(bold** the authors belonging to the project teams and denote the corresponding author with an asterisk*)*	Title and Journal/ Book *(with the volume, pages and other necessary publishing details specified)*	Submitted to RGC *(indicate the year ending of the relevant progress report)*	Attached to this report *(Yes or No)*	Acknowledged the support of this Joint Research Scheme *(Yes or No)*	Accessible from the institutional repository *(Yes or No)*
Year of publication	Year of Acceptance *(For paper accepted but not yet published)*	Under Review	Under Preparation *(optional)*						
2017 (Ref. 1)				**Hang Yin, Sin Hang Cheung, Jenner H. L. Ngai, Carr Hoi Yi Ho, Ka Lok Chiu, Xiaotao Hao**, Ho Wa Li, Yuanhang Cheng, Sai Wing Tsang and **S.K. So***	"Thick-Film High-Performance Bulk-Heterojunction Solar Cells Retaining 90% PCEs of the Optimized Thin Film Cells", Adv. Electr. Mater. **3**, 1700007 (2017).		Y	Y	
2018 (Ref. 2)				**H. Yin, J.K.W. Ho, S.H. Cheung, R.J. Yan, K.L. Chiu, X.T. Hao, and S.K. So***	"Designing a Ternary Photovoltaic Cell for Indoor Light Harvesting with a Power Conversion Efficiency Exceeding 20%", J. Mater. Chem. A, **6**, 8579-8585 (2018)	Y	Y	Y	

2019 (Ref. 3)				**H. Yin, Ka Lok Chiu, Pengqing Bi**, Gang Li, Cenqi Yan, Hua Tang, **Chujun Zhang**, Yiqun Xiao, Hengkai Zhang, Wei Yu, Hanlin Hu, Xinhui Lu, **Xiaotao Hao***, and **S.K. So***	"Enhanced Electron Transport and Heat Transfer Boost Light Stability of Ternary Organic Photovoltaic Cells Incorporating Non-Fullerene Small Molecule and Polymer Acceptors", Adv. Electron. Mater. **5** 1900497 (2019)		Y	Y	
2018 (Ref. 4)				**Hang Yin, Pengqing Bi, Sin Hang Cheung, Wai Leong Cheng, Ka Lok Chiu, Carr Hoi Yi Ho**, Ho Wa Li, Sai Wing Tsang, **Xiaotao Hao, S.K. So***	"Balanced Electric Field Dependent Mobilities: A Key to Access High Fill Factors in Organic Bulk Heterojunction Solar Cells", Solar RRL 2, 1700239 (2018).		Y	Y	
2019 (Ref. 5)				**H. Yin, Jie Yan, Johnny Ka Wai Ho,** Delong Liu, **Pengqing Bi, Carr Hoi Yi Ho, Xiaotao Hao,** Jianhui Hou, Gang Li, **and S.K. So***	"Observing electron transport and percolation in selected bulk heterojunctions bearing fullerene derivatives, non-fullerene small molecules, and polymeric acceptors", , Nano Energy 64, 103950 (2019)		Y	Y	

2018 (Ref. 6)				**Pengqing Bi**, **Tong Xiao, Xiaoyu Yang, Mengsi Niu, Zhenchuan Wen, Kangning Zhang, Wei Qin, S.K. So, Guanghao Lu, Xiaotao Hao*,** Hong Liu	"Regulating the vertical phase distribution by fullerene-derivative in high performance ternary organic solar cells", Nano Energy **46**, 81-90 (2018).		Y	Y	
2019 (Ref. 7)				**Peng Qing Bi**, Christopher R. Hall, **Hang Yin, Shu Kong So**, Trevor A. Smith, Kenneth P. Ghiggino, and **Xiao Tao Hao***	"Resolving the Mechanisms of Photocurrent Improvement in Ternary Organic Solar Cells", *J. Phys. Chem. C* 123, 18294 (2019).		Y	Y	
2020 (Ref. 8)				**Kang-Ning Zhang, Meng-Si Niu, Zhi-Nan Jiang, Zhi-Hao Chen, Tong Wang, Meng-Meng Wei, Chao-Chao Qin, Lin Feng, Wei Qin, Shu-Kong So, Xiao-Tao Hao***	"High-Performance Ternary Organic Solar Cells with Morphology-Modulated Hole Transfer and Improved Ultraviolet Photostability", Solar RRL **4**, 2000165 (2020).		Y	Y	
2021 (Ref. 9)				**Kang-Ning Zhang, Zhi-Nan Jiang, Tong Wang, Jia-Wei Qiao, Lin Feng, Chao-Chao Qin, Hang Yin, Shu-Kong So, Xiao-Tao Hao***	"Exploring the mechanisms of exciton diffusion improvement in ternary polymer solar cells: From ultrafast to ultraslow temporal scale", Nano Energy **79**, 105513 (2021)		Y	Y	

2020 (Ref. 10)				**Kang-Ning Zhang, Meng-Si Niu, Zhi-Nan Jiang, Zhi-Hao Chen, Tong Wang, Meng-Meng Wei, Chao-Chao Qin, Lin Feng, Wei Qin, Shu-Kong So, Xiao-Tao Hao***	"Multiple Temporal-Scale Photocarrier Dynamics Induced by Synergistic Effects of Fluorination and Chlorination in Highly Efficient Nonfullerene Organic Solar Cells", Solar RRL **4**, 1900552 (2020)		Y	Y	

9. Recognized international conference(s) in which paper(s) related to this research project was/were delivered

(Please attach a copy of each delivered paper. All listed papers must acknowledge RGC's funding support by quoting the specific grant reference.)

Month/Year/ Place	Title	Conference Name	Submitted to RGC *(indicate the year ending of the relevant progress report)*	Attached to this report *(Yes or No)*	Acknowledged the support of this Joint Research Scheme *(Yes or No)*	Accessible from the institutional repository *(Yes or No)*
Nov/2019	Electron transport and percolation in bulk-heterojunctions bearing different classes of electron acceptors	TF-POE2019 Shandong U	N	Y	Y	
Dec/2018/ Shenzhen, China	Designing photovoltaic cells for room light harvesting	12th Aseanian Conference on Nano-hybrid Solar Cells (NHSC), Shenzhen	Y (Dec 2018)	Y	Y	
Aug/2017 San Diego, USA	Thick-Film High-Performance Bulk-Heterojunction Solar Cells Retaining 90% PCEs of the Optimized Thin Film Cells	Society for Photonics and Information Engineering (SPIE) Photonic West, San Diego, USA	Y (Dec 2018)	Y	Y	

10. Student(s) trained *(Please attach a copy of the title page of the thesis.)*

Name	Degree registered for	Date of registration	Date of thesis submission/ graduation
YIN Hang	PhD (HKBU)	1/9/2014	Aug 2017
CHEUNG Sin Hang	MPhil (HKBU)	1/9/2016	May 2019
BI Pengqing	PhD (SDU)	6/9/2014	May 2019

11. Other impact *(e.g. award of patents or prizes, collaboration with other research institutions, technology transfer, etc.)*

The jointly trained PhD student, Dr Yin Hang, made notable contributions to this project and impacts to the field. In 2020, he joint the School of Physics in Shandong U, and is expected to combined strengths from both sides to make new discoveries in organic electronics.

12. Statistics on Research Outputs *(Please ensure the summary statistics below are consistent with the information presented in other parts of this report.)*

	Peer-reviewed journal publications	Conference papers	Scholarly books, monographs and chapters	Patents awarded	Other research outputs (Please specify)
No. of outputs arising directly from this research project [or conference]	10 (IF>10, 4 papers; 10 > IF >6, 5 papers)	3			