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

Development of Polymer/Polymer-Blend-Based Bulk-Heterojunction Organic Photovoltaics

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

	Hong Kong Team	Mainland Team
Name of Principal	Prof. He YAN	Prof. Fei Huang
Investigator (with title)		
Post	Associate Professor	Professor
Unit / Department / Institution	Department of Chemistry/Hong Kong University of Science and Technology	School of Materials Science and Engineering, South China University of Technology
Contact Information	hyan@ust.hk	msfhuang@scut.edu.cn
Co-investigator(s) (with title and institution)		

3. Project Duration

	Original	Revised	Date of RGC/ Institution Approval (must be quoted)
Project Start date	Jan 1 st 2014		
Project Completion date	Dec 31 st 2017		
Duration (in month)	48		
Deadline for Submission of Completion Report	Dec 31 st 2018		

Part B: The Completion Report

5. Project Objectives

5.1 Objectives as per original application

1. The Hong Kong PI will develop n-type semiconducting polymers for PP-OPVs. Our previously reported n-type polymer, P(NDI-2OD-T2), was designed for the organic transistor that has somewhat different requirements from PP-OPVs. In the project, our goal is to develop n-type polymers that will enable efficient PP-OPVs

2. The Mainland PI will develop p-type semiconducting polymers for PP-OPVs. We will develop p-type polymers that match with the n-type polymers in energy levels and processing properties. 3. We will integrate the n-type and p-type polymers to construct PP-OPVs. Our goal is to achieve 7% efficiency PP-OPVs and to understand the relationship between the chemical structures of the polymers and device performances of the PP-OPVs.

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)

1. Developed all-polymer solar cells with 8.59% efficiency.

A new polymer acceptor, naphthodiperylenetetraimide-vinylene (NDP-V), featuring a backbone of altenating naphthodiperylenetetraimide and vinylene units is designed and applied in all-polymer solar cells (all-PSCs). With this polymer acceptor, a new record power-conversion efficiencies (PCE) of 8.59% has been achieved for all-PSCs.

2. Developed non-fullerene polymer solar cells with 7.3% efficiency.



Figure 1. Stucture of PffT2-FTAZ-2DT and IEIC

We have designed and synthesized a large-bandgap ($E_g \sim 1.91 \text{ eV}$) polymer PffT2-FTAZ-2DT based on the difluoro-triazole unit which structure is shown in Figure 1. We found that, the polymer PffT2-FTAZ-2DT could form complementary absorption with a small-bandgap acceptor IEIC which will broaden the absorption range of the active layer to 400-800 nm. In fact, non-fullerene solar cell based on PffT2-FTAZ-2DT and IEIC could achieve a high power conversion efficiency of 7.3% which is among the highest efficiencies at that time. Other characterization results indicate that balanced hole and electron mobility, face-on polymer chain orientation and highly efficient charge transfer and transport process are the reasons for the relatively high fill factor of 0.59. Also, the temperature dependent aggregation property of PffT2-FTAZ-2DT ensures a suitable domain size and phase separation. This work successfully illustrates the effectiveness of the strategy and provides important guidance of designing high-performance electron acceptors.

3. Developed fast charge separation in a non-fullerene organic solar cell with a small driving force.



Figure 2. Stucture of P3TEA and SF-PDI₂

we reported non-fullerene OSCs that exhibit ultrafast and efficient charge separation despite a negligible driving force, as ECT is nearly identical to E_{gap} . Moreover, the small driving force is found to have minimal detrimental effects on charge transfer dynamics of the OSCs. We demonstrate a non-fullerene OSC with 9.5% efficiency and nearly 90% internal quantum efficiency despite a low voltage loss of 0.61V. This creates a path towards highly efficient OSCs with a low voltage loss.

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

For further development, extensive research efforts should be spent on new donor and acceptor materials design. More specifically, as the morphological stability of the active layers plays a crucial issue for future large-scale roll-to-roll production, much research effort

should be devoted to controlling the aggregation behavior of the polymer chains and the blend film morphology by developing new polymer acceptors, regulating the molecular weights of the polymer donors or acceptors and optimizing film deposition conditions, including the processing solvents and solvent additives used. In addition, studies on the charge generation and separation process in PP-PSCs are also necessary for gain deep understanding in organic semiconductors and also guide the new materials design.

7. The Layman's Summary

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

As an emerging technology for harnessing solar energy, polymer solar cells (PSCs) have received extensive attention during the past decade. The appealing properties of solution-processed PSCs include low cost, light weight, mechanical flexibility, and promise of facile large-area fabrications. Compared to fullerene- and small molecule-based devices, all-PSCs offer additional merits of high morphological stability, superior mechanical properties, and suitability for printing-related fabrication techniques. In this project, we started from both polymer donor and acceptor materials design, and achieved PP-PSCs with power conversion efficiency over 10%. The project helps us developing a series of design strategies for high performance materials. In the meanwhile, we carried out some fundamental studied from the charge generation in the non-fullerene PSCs and gain more deep understanding in the PSC filed. We also revealed the quantitative relations between interaction parameter, miscibility and function in PSCs, which ensure us a facile way of fine tuning the active layer morphology in PSCs and achieve high power conversion efficiency.

Part C: Research Output

8. Peer-reviewed journal publication(s) arising <u>directly</u> 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	e Latest Status	of Publica	tions	Author(s)	Title and	Submitted to	Attached	Acknowledge	Accessible
Year of	Year of	Under	Under	(bold the	Journal/	RGC	to this	d the support	from the
publication	Acceptance	Review	Preparation	authors	Book	(indicate the	report (Yes	of this Joint	institutional
^	(For paper		-	belonging to	(with the	year ending	or No)	Research	repository
	accepted but		(optional)	the project	volume,	of the		Scheme	(Yes or No)
	not yet			teams and	pages and	relevant		(Yes or No)	
	published)			denote the	other	progress			
				corresponding	necessary	report)			
				author with an	publishing				
				asterisk*)	details				
					specified)				

2014		Mu, C., Liu, P., Ma, W.*, Jiang, K., Zhao, J., Zhang, K., Chen, Z., Wei, Z., Yi, Y., Wang, J., Yang, S., Huang, F.*, Facchetti, A.,	High-Effici ency All-Polyme r Solar Cells Based on a Pair of Crystalline Low-Band gap Polymers".	31-Dec-2 015	NO	Yes	Yes
		Ade, H.*, Yan, H.*	Advanced Materials, (2014), 26(42), 7224-7230				
2015		Lin, H., Chen, S., Li, Z., Lai, J.Y.L., Yang, G., McAfee, T., Jiang, K., Li, Y., Liu Y., Hu, H., Zhao, J., Ma, W., Ade, H., Yan, H.*	High-Perfo rmance Nonfullere ne Polymer Solar Cells Based on a Pair of Donor-Acc eptor Materials with Compleme ntary Absorption Properties. " Advanced Materials, (2015), published online, DOI:10.10 02/adma20 1502775.	31-Dec-2 015	NO	Yes	Yes

2015		Hu, H., Jiang K., Yang G., Liu J., Li, Z., Lin, H., Liu Y., Zhao J., Zhang J., Huang, F., Qu, Q., Ma W.*, Yan H.*	Terthiophe ne-based D-A polymer with an asymmetri c arrangeme nt of alkyl chains that enables efficient polymer solar cells." <i>Journal of the</i> <i>American</i> <i>Chemical</i> <i>Society</i> , (2015), published online, DOI :10.10 21/jacs.5b0	31-Dec-2 015	NO	Yes	Yes
2016		Yikun Guo , Yunke Li , Omar Awartani , Jingbo Zhao , Han Han , Harald Ade , * Dahui Zhao , * and He Yan *	A Vinylene- Bridged Perylenedii mide-Base d Polymeric Acceptor Enabling Effi cient All-Polym er Solar Cells Processed under Ambient Conditions <i>Adv.</i> <i>Mater.</i> 2016, 28, 8483–8489	31-Dec-20 18	Yes	Yes	Yes

2017		Yikun Guo,	Improved	31-Dec-20	Yes	Yes	Yes
		Yunke Li,	Performan	18			
		Omar	ce of				
		Awartani,	All-Polym				
		Han Han,	er Solar				
		Jingbo Zhao,	Cells				
		Harald Ade,*	Enabled				
		He Yan,*	by				
		and Dahui	Naphthodi				
		Zhao*	perylenetet				
			raimide-Ba				
			sed				
			Polymer				
			Acceptor				
			Adv.				
			Mater.				
			2017, 29,				
			1700309				
	2018	Huatong	Efficient	31-Dec-20	Yes	Yes	No
		Yao, Fujin	All-Polym	18			
		Bai, Huawei	er Solar				
		Hu,	Cells based				
		Lingeswaran	on a Novel				
		Arunagiri,	Polymer				
		Jianquan	Acceptor				
		Zhang,	Achieving				
		Yuzhong	10.3%				
		Chen,	Power				
		Shangshang	Conversion				
		Chen, Tao,	Efficiency				
		Liu, Joshua	A du				
		Yuk Lin Lai,	AUV. Energy				
		Harald	Mator				
		Ade,*and He	maier.				
		Yan*					

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/	Title	Conference Name	Submitted	Attached	Acknowledged	Accessible
Place			to RGC	to this	the support of	from the
			(indicate the	report	this Joint	institutional
			year ending	(Yes or No)	Research	repository
			of the		Scheme	(Yes or No)
			relevant		(Yes or No)	
			progress		, í	
			report)			

None

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
Jingbo Zhao	PhD	Sep 2012	Dec 2015

Huatong Yao	PhD	Feb. 2016	Dec 2019

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

Full list of publications directly generated by this project.

- 1. Yikun Guo, Yunke Li, Omar Awartani, Jingbo Zhao, Han Han, Harald Ade, * Dahui Zhao, * and He Yan * "A Vinylene-Bridged Perylenediimide-Based Polymeric Acceptor Enabling Effi cient All-Polymer Solar Cells Processed under Ambient Conditions" Adv. Mater. (2016), 28, 8483–8489
- 2. Yikun Guo, Yunke Li, Omar Awartani, Han Han, Jingbo Zhao, Harald Ade,* He Yan,* and Dahui Zhao* "Improved Performance of All-Polymer Solar Cells Enabled by Naphthodiperylenetetraimide-Based Polymer Acceptor" Adv. Mater. (2017), 29, 1700309