

University of Groningen

## Conjugated molecules

Ye, Gang

**IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.**

*Document Version*

Publisher's PDF, also known as Version of record

*Publication date:*

2019

[Link to publication in University of Groningen/UMCG research database](#)

*Citation for published version (APA):*

Ye, G. (2019). *Conjugated molecules: Design and synthesis of 羰基-conjugated materials for optoelectronic and thermoelectric applications.*

### Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

### Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

*Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.*

# **CONJUGATED MOLECULES**

Design and synthesis of  $\pi$ -conjugated materials for  
optoelectronic and thermoelectric applications

**Gang Ye**



university of  
 groningen

faculty of science  
 and engineering

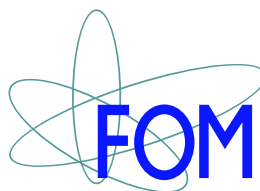
## CONJUGATED MOLECULES

Design and synthesis of  $\pi$ -conjugated materials for optoelectronic and thermoelectric applications

Gang Ye

This project was carried out in the research group Chemistry of (Bio)Molecular Materials and Devices which is part of Stratingh Institute for Chemistry and Zernike Institute for Advanced Materials, University of Groningen, The Netherlands.

This work was funded by China Scholarship Council. This work is part of the research program of the Foundation for Fundamental Research on Matter (FOM), which is part of The Netherlands Organization for Scientific Research (NWO).



*Printed by:* GVO drukkers & vormgevers B.V.

*Front & Back:* The cover is designed by Gang Ye.

Copyright © 2019 by G. Ye

ISBN: 978-97-034-1659-5 (printed)

ISBN: 978-94-034-1658-8 (electronic)

An electronic version of this dissertation is available at

<http://www.rug.nl/research/portal>.



university of  
 groningen

## **CONJUGATED MOLECULES**

Design and synthesis of  $\pi$ -conjugated materials for  
 optoelectronic and thermoelectric applications

### **PhD Thesis**

to obtain the degree of PHD at the  
 University of Groningen  
 on the authority of the  
 Rector Magnificus Prof. E. Sterkrn  
 and in accordance with  
 the decision by the College of Deans.

This thesis will be defended in public on

Friday 14 June 2019 at 9:00 hours

by

**Gang Ye**

born on 12 June 1986  
 in Hubei, China.

**Supervisors**

Prof. R.C. Chiechi

Prof. J.C. Hummelen

**Assessment Committee**

Prof. K.U. Loos

Prof. M.M.G. Kamperman

Prof. H. Zhang

*To my dear family*



# Contents

<b>1</b>	<b>Introduction</b>	<b>1</b>
1.1	The Field of Conjugated Polymers and Organic Electronics Applications . . . . .	2
1.2	Intrinsic Conjugated Polymers and Polymer Solar Cells . . . . .	2
1.3	Doped Conjugated Polymers and Thermoelectric Devices . . . . .	6
1.4	General Routes for Synthesis of Conjugated Polymers . . . . .	11
1.5	Green Solvents Processable Conjugated Polymers . . . . .	13
1.6	Thesis Outline . . . . .	15
	References . . . . .	17
<b>2</b>	<b>Synthesis, Optical and Electrochemical Properties of High-quality Cross-conjugated Aromatic Polyketones</b>	<b>25</b>
2.1	Introduction . . . . .	26
2.2	Results and Discussion . . . . .	27
2.2.1	Synthesis and Characterization . . . . .	27
2.2.2	Thermal Properties . . . . .	28
2.2.3	Photophysical Properties . . . . .	30
2.2.4	Electrochemical Properties . . . . .	32
2.2.5	Density Functional Theory Calculation . . . . .	33
2.3	Conclusion . . . . .	34
2.4	Experimental . . . . .	34
	References . . . . .	41
<b>3</b>	<b>Conjugated Polyions Enable Organic Photovoltaics Processed from Green Solvents</b>	<b>43</b>
3.1	Introduction . . . . .	44
3.2	Results and Discussion . . . . .	45
3.2.1	Synthesis and Characterization . . . . .	45
3.2.2	Photophysical Properties . . . . .	46
3.2.3	Electrochemical Properties . . . . .	48
3.2.4	Density Functional Theory Calculation . . . . .	48
3.2.5	Device Characteristic . . . . .	48
3.3	Conclusion . . . . .	52
3.4	Experimental . . . . .	52
	References . . . . .	64



<b>4</b>	<b>The Effects of Ethylene Glycol Side Chains on Molecular N-doping of Low Bandgap Donor-Acceptor Copolymers</b>	<b>69</b>
4.1	Introduction . . . . .	70
4.2	Results and Discussion . . . . .	71
4.3	Conclusions . . . . .	81
4.4	Experimental . . . . .	81
4.4.1	Device Fabrication and Characterization . . . . .	82
4.4.2	Synthesis and Characterization . . . . .	85
	References . . . . .	89
<b>5</b>	<b>N-type Organic Thermoelectrics of Donor-Acceptor Copolymers: Improved Power Factor by Molecular Tailoring of the Density of States</b>	<b>93</b>
5.1	Introduction . . . . .	94
5.2	Results and Discussions . . . . .	95
5.3	Conclusions . . . . .	102
5.4	Experimental . . . . .	102
5.4.1	Synthesis and Characterization of Materials. . . . .	102
5.4.2	General Synthetic Procedures for the NDI Based D-A Copolymers . . . . .	103
5.4.3	Characterization of NDI Based D-A Copolymers. . . . .	105
5.4.4	Device Fabrication and Characterization . . . . .	107
	References . . . . .	116
<b>6</b>	<b>Molecular Wires Conductance: Linear Conjugation versus Cross Conjugation</b>	<b>121</b>
6.1	Introduction . . . . .	122
6.2	Results and Discussion . . . . .	123
6.2.1	Design and Synthesis of Molecular Wires . . . . .	123
6.2.2	UV-Vis Absorption Spectroscopy . . . . .	126
6.2.3	Conductance Measurements . . . . .	127
6.2.4	Transport Calculation . . . . .	131
6.3	Conclusions . . . . .	135
6.4	Experimental . . . . .	136
	References . . . . .	145
	<b>Summary</b>	<b>151</b>
	<b>Samenvatting</b>	<b>155</b>
	<b>Acknowledgements</b>	<b>159</b>