Electronic Structure of Organic Semiconductors

Polymers and small molecules

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Morgan & Claypool Publishers

ISBN 978-1-64327-168-2 (ebook)
ISBN 978-1-64327-165-1 (print)
ISBN 978-1-64327-166-8 (mobi)

DOI 10.1088/2053-2571/aaddd8

Version: 20181201

IOP Concise Physics
ISSN 2053-2571 (online)
ISSN 2054-7307 (print)

A Morgan & Claypool publication as part of IOP Concise Physics
Published by Morgan & Claypool Publishers, 1210 Fifth Avenue, Suite 250, San Rafael, CA, 94901, USA

IOP Publishing, Temple Circus, Temple Way, Bristol BS1 6HG, UK

To my Research Group

Contents

Preface x

Acknowledgements xi

Author biography xii

Fundamental constants xiii

Greek alphabet xiv

1 Introduction 1-1

References 1-2

2 Some basic concepts in solid state physics 2-1

2.1 Drude model 2-1

2.1.1 AC conductivity and optical properties of a metal 2-3

2.1.2 Electronic polarizability and permittivity 2-4

2.2 Sommerfeld model 2-7

2.2.1 Excited states of the Fermi gas: electrons and holes 2-11

Further reading 2-11

Problems 2-11

References 2-12

3 From orbitals to bands 3-1

3.1 Orbitals in a chain of atoms 3-1

3.2 Importance of the crystal structures 3-4

3.2.1 Bravais lattices 3-4

3.2.2 Reciprocal space: reciprocal lattice and Brillouin zone 3-5

3.3 Covalent solids: the series C, Si, Ge 3-7

Further reading 3-9

Problems 3-9

References 3-9

4 Band theory 4-1

4.1 Electrons in a periodic potential: Bloch theorem 4-1

4.2 Energy bands from linear combinations of orbitals 4-5

4.2.1 One orbital per primitive cell 4-5

4.2.2 More than one orbital per primitive cell 4-8

4.3 Energy bands in a one-dimensional crystal 4-9
4.3.1 One atom per primitive cell 4-9
4.3.2 Two atoms per primitive cell 4-10
4.3.3 Instabilities in one-dimensional solids: Peierls transition 4-11
4.4 Consequences of the band structure in semiconductors 4-13
4.4.1 Dynamics of electrons and holes 4-13
4.4.2 Density of charge carriers (electrons and holes) 4-15
Further reading 4-17
Problems 4-17
References 4-18

5 Orbitals and bands in organic semiconductors 5-1

5.1 Energy bands in conjugated polymers 5-6
5.1.1 Energy bands in polyacetylene 5-7
5.1.2 Energy bands in poly(p-phenylene vinylene) (PPV) 5-8
5.2 Electronic structure of small molecule organic semiconductors 5-9
Problems 5-12
References 5-12

6 Computational methods 6-1

6.1 Hartree–Fock theory 6-1
6.2 Density functional theory (DFT) 6-5
6.2.1 Ionization potential, electron affinity and energy gaps 6-8
6.3 Molecular orbitals calculated by DFT 6-10
6.3.1 Small molecules 6-12
6.4 Energy bands calculated by DFT 6-15
6.4.1 Band structure of poly(p-phenylene vinylene) (PPV) 6-16
6.4.2 Band structure of pentacene 6-18
Further reading 6-19
Problems 6-19
References 6-20

7 Topological defects and excitons 7-1

7.1 Topological defects: solitons and polarons 7-1
7.2 Electron–hole interactions: excitons 7-3
7.2.1 Ground state and excited states 7-4

7.2.2 Wannier excitons 7-6
7.2.3 Frenkel excitons 7-8
Further reading 7-13
Problems 7-13
References 7-14

8 Transport and optical properties 8-1
8.1 Transport properties 8-1
8.1.1 Hopping transport 8-2
8.1.2 Transport via polaron hopping 8-3
8.2 Optical properties 8-4
Further reading 8-9
Problems 8-9
References 8-10

9 Case study: PEDOT:PSS 9-1
9.1 Introduction 9-1
9.2 Electronic structure 9-2
9.3 Electronic and optical properties 9-7
9.4 Approaches to improve the electrical conductivity 9-9
9.5 Applications 9-12
Further reading 9-12
Problems 9-13
References 9-13

Appendix A A-1

Appendix B B-1

Preface

This ebook originated in a series of lectures on the electronic structure of organic semiconductors prepared for a training European network in the field of organic solar cells and expanded for the use of researchers of the Organic Electronics Group at IT/Lisbon. It was written from the perspective of an experimental chemist and intends to put together some fundamentals from chemistry, solid state physics and quantum chemistry, to help understand and predict the electronic and optical properties of organic semiconductors, polymers and small molecules. The text is intended to assist graduate students and researchers of different backgrounds to use theory to design more efficient materials for organic electronic devices, such as organic solar cells, light emitting diodes, field effect transistors and sensors. After addressing some basic topics in solid state physics, a comprehensive introduction to molecular orbitals and band theory leads to a description of computational methods based on Hartree–Fock and density functional theory, for predicting geometry conformations, frontier levels and energy band structures. Topological defects and transport and optical properties are then addressed, and one of the most commonly used transparent conducting polymers, PEDOT:PSS, is described in some detail as a case study.

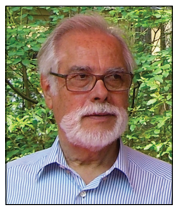
Luís Alcácer
August 2018

Acknowledgements

I wish to express my gratitude to my co-workers of the Organic Electronics Group and to my institution, the Instituto de Telecomunicações, for their support in the preparation of this text, to my colleagues Jorge Morgado, Ana Charas and Henrique Gomes for reading the quasi-final draft and their suggestions, and finally to Nicki Dennis and Karen Donnison at IOP Concise Physics for their assistance in the preparation of the manuscript into its final form.

Author biography

Luís Alcácer



Luís Alcácer obtained his PhD from the University of California, Riverside, in 1970. He held a research position at the Nuclear Physics and Engineering Laboratory in Portugal and in 1975 became Full Professor at Instituto Superior Técnico (IST-Universidade de Lisboa), where he lectured in the areas of Chemical Physics, Solid State Physics and Quantum Mechanics. He is now Emeritus Professor at IST and a senior researcher at Instituto de Telecomunicações. His research interests have been focused on organic conductors and semiconductors, polymer electrolytes and organic electronics. He is the author of 'Introduction to Quantum Mechanics with Applications to Modern Computational Chemistry', IST Press, 2007, 2014 (in Portuguese). He also authored 'The Devil in the Quantum World', Gradiva, 2013 (in Portuguese), a book about the mysteries of quantum mechanics. His curriculum vitae may be seen at https://www.it.pt/Members/Index/359.

Fundamental constants

Constant	Symbol	Value	Units
Velocity of light in vacuum	c	299 792 458	m s^{-1}
Planck's constant	h	$6.626\ 070\ 040 \times 10^{-34}$	J s
$\hbar = h/2\pi$	$\hbar$	$1.054\ 571\ 800 \times 10^{-34}$	J s
Elementary charge	e	$1.602\ 176\ 6208 \times 10^{-19}$	C
Vacuum permittivity	ε_0	$8.854\ 187\ 817\cdots\times10^{-12}$	F m^{-1}
Electron mass	m_e	$9.109\ 383\ 56 \times 10^{-31}$	kg
Proton mass	m_p	$1.672\ 621\ 898 \times 10^{-27}$	kg
Boltzmann's constant	k	$1.380\ 648\ 52 \times 10^{-23}$	J K^{-1}
		$8.617\ 3303 \times 10^{-5}$	eV K^{-1}
Avogadro number	N_A	$6.022\ 140\ 857 \times 10^{23}$	mol^{-1}
Bohr radius, $a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2}$	a_0	$0.529\ 177\ 210\ 67 \times 10^{-10}$	m
	$1\ eV$	$1.602\ 176\ 6208 \times 10^{-19}$	J

Note: The values in the table are those recommended by CODATA 2014 (CODATA is the acronym of 'Committee on Data for Science and Technology'). See http://physics.nist.gov/cuu/Constants/index.html.

Greek alphabet

A	α	Alpha	N	ν	Nu
B	β	Beta	Ξ	ξ	Xi
Γ	γ	Gamma	*O*	o	Omicron
Δ	δ	Delta	Π	π	Pi
E	ϵ	Epsilon	P	ρ	Rho
Z	ζ	Zeta	∑	σ	Sigma
H	η	Eta	T	τ	Tau
Θ	θ	Theta	ϒ	υ	Upsilon
I	ι	Iota	Φ	ϕ	Phi
K	κ	Kappa	X	χ	Chi
Λ	λ	Lambda	Ψ	ψ	Psi
M	μ	Mu	Ω	ω	Omega