

Contents

Acknowledgements — V

Abstract — VII

Introduction — 1

1 Organic Semiconductor Devices — 9

- 1.1 Solar Cells — 9
- 1.2 Light Emitting Diodes — 12
- 1.3 Field Effect Transistors — 17
- 1.4 Lasers — 18

2 Experimental Techniques — 21

- 2.1 Mobility Measurements — 21
- 2.2 Charge Density Measurements — 27
- 2.3 Doping — 30

3 Charge Dynamics at Different Scales — 34

- 3.1 Charge Transfer Reactions — 35
- 3.2 Band Theory vs. Hopping Transport — 40
- 3.3 Stochastic Description of Hopping Transport in Discrete Space — 41
- 3.4 Kinetic Monte Carlo — 45
- 3.5 Differential Equation Solver — 54
- 3.6 Gaussian Disorder Models — 55
- 3.7 Analytic Theories of Hopping Transport — 58
- 3.8 Continuous Space Charge Transport — 65
- 3.9 Heuristic Models — 67

4 Computational Methods — 70

- 4.1 Density Functional Theory — 71
- 4.2 Molecular Dynamics — 73
- 4.3 Electrostatic and Induction Calculations for Site Energies — 77
- 4.4 Coarse-Grained Morphology — 78

5 Energetics and Dispersive Transport — 83

- 5.1 Methods — 84
- 5.2 Scaling Relation — 85
- 5.3 Finite Carrier Density — 90
- 5.4 Conclusions — 93

6	Correlated Energetic Landscapes — 94
6.1	Atomistic Simulations — 95
6.2	The Algorithm — 98
6.3	Validation — 101
7	Microscopic, Stochastic and Device Simulations — 104
7.1	Microscopic Modeling — 107
7.2	Coarse-Grained Models — 112
7.3	Lattice Models — 117
7.4	Charge Dynamics — 119
7.5	Device Simulations — 121
7.6	Experiment — 126
7.7	Materials — 127
8	Parametrization of Lattice Models — 131
8.1	Methodology — 132
8.2	Results — 135
8.3	Conclusions — 138
8.4	Supporting Information — 139
9	Drift–Diffusion with Microscopic Link — 143
9.1	Methods — 144
9.2	Validation — 151
9.3	Conclusions — 152
Conclusions and Outlook — 153	
A	Molecule Abbreviations — 156
Bibliography — 157	
Index — 189	