

# Contents

List of Contributors		xvi
<b>1 Nanoelectronic devices: A unified view</b>		<b>1</b>
<i>Supriyo Datta</i>		
1.1 Introduction		1
1.2 The NEGF–Landauer model		5
1.3 A few examples		12
1.4 Concluding remarks		19
References		21
<b>2 Electronic and transport properties of doped silicon nanowires</b>		<b>23</b>
<i>M.-V. Fernández-Serra and X. Blase</i>		
2.1 Introduction		23
2.2 Electronic structure of silicon nanowires		24
2.3 Doping characteristics of SiNWs		26
2.4 Electronic transport		30
2.5 Multiple impurities and disorder		36
2.6 Covalent functionalization of SiNWs		37
2.7 Conclusions		42
References		43
<b>3 NEGF-based models for dephasing in quantum transport</b>		<b>46</b>
<i>Roksana Golizadeh-Mojarad and Supriyo Datta</i>		
3.1 Introduction		46
3.2 Dephasing model		47
3.3 Effect of different types of dephasing on momentum and spin relaxation		48
3.4 Effect of different types of dephasing on phase relaxation		50
3.5 Calculating $L_m$ , $L_s$ , and $L_\varphi$		51
3.6 Example: “spin-Hall” effect		55
3.7 Summary		60
References		60
<b>4 Molecular nanowires and their properties as electrical conductors</b>		<b>62</b>
<i>George Kirczenow</i>		
4.1 Introduction		62
4.2 What are molecular nanowires?		63
4.3 Molecular nanowires have been realized in a variety of ways		65

4.4	A major challenge: The atomic-scale geometry is not known	67
4.5	Brief overview of molecular nanowire varieties: Different molecules, linkers and electrodes	70
4.6	Electrical conduction as a quantum scattering problem	75
4.7	Model building: Principles and caveats	79
4.8	Theory confronts experiment: Some case studies	88
4.9	Summary and outlook	99
	Acknowledgments	103
	References	104
<b>5</b>	<b>Quasi-ballistic electron transport in atomic wires</b>	<b>117</b>
	<i>Jan M. van Ruitenbeek</i>	
5.1	Introduction	117
5.2	Experimental techniques	118
5.3	Atomic-sized metallic contacts	121
5.4	Metal–molecule–metal junctions	133
5.5	Conclusion	140
	References	140
<b>6</b>	<b>Thermal transport of small systems</b>	<b>145</b>
	<i>Takahiro Yamamoto, Kazuyuki Watanabe, and Satoshi Watanabe</i>	
6.1	Introduction	145
6.2	Boltzmann–Peierls formula of diffusive phonon transport	146
6.3	Coherent phonon transport	149
6.4	Quasi-ballistic phonon transport	158
6.5	Conclusions	163
	Acknowledgments	164
	Appendix: Derivation of eqn (6.42)	165
	References	165
<b>7</b>	<b>Atomistic spin-dynamics</b>	<b>167</b>
	<i>M. Stamenova and S. Sanvito</i>	
7.1	Introduction	167
7.2	Model spin Hamiltonian	169
7.3	Test simulations	171
7.4	Current-induced domain-wall motion	186
7.5	Spin-motive force	203
7.6	Conclusions	210
	Acknowledgments	210
	References	211
<b>8</b>	<b>Patterns and pathways in nanoparticle self-organization</b>	<b>214</b>
	<i>MO Blunt, A. Stannard, E. Pauliac-Vaujour, CP Martin, Ioan Vancea, Milovan Šuvakov, Uwe Thiele, Bosiljka Tadić, and P. Moriarty</i>	
8.1	Introduction	214
8.2	Self-assembled and self-organized nanoparticle arrays	215

8.3	Pathways for charge transport in nanoparticle assemblies	237
8.4	Conclusion	245
	Acknowledgments	245
	References	245
<b>9</b>	<b>Self-organizing atom chains</b>	<b>249</b>
	<i>Arie van Houselt and Harold J.W. Zandvliet</i>	
9.1	Introduction	249
9.2	Formation of monoatomic Pt chains on Ge(001)	255
9.3	Quantum confinement between monoatomic Pt chains	263
9.4	Peierls instability in monoatomic Pt chains	269
9.5	Conclusions and outlook	275
	References	276
<b>10</b>	<b>Designing low-dimensional nanostructures at surfaces by supramolecular chemistry</b>	<b>278</b>
	<i>Nian Lin and Sebastian Stepanow</i>	
10.1	Introduction	278
10.2	Hydrogen-bond systems	281
10.3	Metal-co-ordination systems	297
10.4	Conclusions	305
	References	305
<b>11</b>	<b>Nanostructured surfaces: Dimensionally constrained electrons and correlation</b>	<b>308</b>
	<i>E. Bertel and A. Menzel</i>	
11.1	Introduction	308
11.2	Motivation	310
11.3	Interactions in low-dimensional systems	317
11.4	Self-assembled nanostructures on surfaces	325
11.5	The phase diagram of real quasi-1D systems	331
11.6	Conclusions	350
	Acknowledgments	351
	References	351
<b>12</b>	<b>Reaction studies on nanostructured surfaces</b>	<b>355</b>
	<i>Adolf Winkler</i>	
12.1	Introduction	355
12.2	Nanostructured surfaces	356
12.3	Fundamentals of reaction processes	361
12.4	Experimental techniques	374
12.5	Selected experimental results	380
12.6	Summary	391
	Acknowledgments	392
	References	392

<b>13 Nanotribology</b>	<b>396</b>
<i>S.K. Biswas</i>	
13.1 Introduction	396
13.2 Nanotribological tools	399
13.3 Interfacial phenomena and interaction forces	401
13.4 Microscopic origin of friction	405
13.5 Oil in confinement and boundary lubrication	415
13.6 Additives in confinement-boundary lubrication	417
13.7 Summary	435
Acknowledgments	437
References	437
<b>14 The electronic structure of epitaxial graphene—A view from angle-resolved photoemission spectroscopy</b>	<b>441</b>
<i>S.Y. Zhou and A. Lanzara</i>	
14.1 Introduction	441
14.2 Electronic structure of graphene	442
14.3 Sample growth and characterization	445
14.4 Electronic structure of epitaxial graphene	447
14.5 Gap opening in single-layer epitaxial graphene	451
14.6 Possible mechanisms for the gap opening	454
14.7 Conclusions	460
Acknowledgments	461
References	461
<b>15 Theoretical simulations of scanning tunnelling microscope images and spectra of nanostructures</b>	<b>464</b>
<i>Jinlong Yang and Qunxiang Li</i>	
15.1 Introduction	464
15.2 Theories of STM and STS	466
15.3 Conventional STM and STS investigations	472
15.4 Beyond conventional STM investigations	489
15.5 Concluding remarks	503
References	503
<b>16 Functionalization of single-walled carbon nanotubes: Chemistry and characterization</b>	<b>508</b>
<i>R. Graupner and F. Hauke</i>	
16.1 Introduction	508
16.2 Chemical functionalization of single-walled carbon nanotubes	509
16.3 Characterization	527
16.4 Conclusion	541
References	541
<b>17 Quantum-theoretical approaches to proteins and nucleic acids</b>	<b>549</b>
<i>Mauro Boero and Masaru Tateno</i>	
17.1 Introduction	549
17.2 Hartree–Fock and all-electron approaches	553

17.3	Density-functional theory approaches	561
17.4	Hybrid QM/MM approaches	576
17.5	Beyond the local-minima exploration	587
17.6	Final remarks	592
	References	592
<b>18</b>	<b>Magnetoresistive phenomena in nanoscale magnetic contacts</b>	<b>599</b>
	<i>J.D. Burton and E.Y. Tsymlal</i>	
18.1	Introduction	599
18.2	Ballistic transport and conductance quantization	603
18.3	Domain-wall magnetoresistance at the nanoscale	611
18.4	Anisotropic magnetoresistance in magnetic nanocontacts	619
18.5	Tunnelling anisotropic magnetoresistance in broken contacts	626
18.6	Conclusions and outlook	629
	Acknowledgments	632
	References	633
<b>19</b>	<b>Novel superconducting states in nanoscale superconductors</b>	<b>639</b>
	<i>A. Kanda, Y. Ootuka, K. Kadowaki, and F.M. Peeters</i>	
19.1	Introduction	639
19.2	Theoretical formalism	642
19.3	Theoretical predictions of vortex states in thin mesoscopic superconducting films	644
19.4	Experimental techniques for detection of vortices	655
19.5	Experimental detection of mesoscopic vortex states in disks and squares	659
19.6	One-dimensional vortex in mesoscopic rings	668
19.7	Conclusion	672
	References	673
<b>20</b>	<b>Left-handed metamaterials—A review</b>	<b>677</b>
	<i>E. Ozbay, G. Ozkan, and K. Aydin</i>	
20.1	Introduction	677
20.2	Negative-permeability metamaterials	678
20.3	Left-handed metamaterial	681
20.4	Negative refraction	684
20.5	Negative phase velocity	687
20.6	Subwavelength imaging and resolution	688
20.7	Planar negative-index metamaterials	691
20.8	Conclusion	698
	Acknowledgments	699
	References	700
<b>21</b>	<b>2D arrays of Josephson nanocontacts and nanogranular superconductors</b>	<b>703</b>
	<i>Sergei Sergeenkov</i>	
21.1	Introduction	703
21.2	Model of nanoscopic Josephson junction arrays	705

21.3	Magnetic-field-induced polarization effects in 2D JJA	710
21.4	Giant enhancement of thermal conductivity in 2D JJA	713
21.5	Thermal expansion of a single Josephson contact and 2D JJA	720
21.6	Summary	726
	Acknowledgments	728
	References	728
<b>22</b>	<b>Theory, experiment and applications of tubular image states</b>	<b>731</b>
	<i>D. Segal, P. Král, and M. Shapiro</i>	
22.1	Introduction	731
22.2	Characterizing tubular image states	734
22.3	Manipulating tubular image states	750
22.4	Experimental verifications	764
22.5	Summary	767
	Acknowledgments	767
	References	767
<b>23</b>	<b>Correlated electron transport in molecular junctions</b>	<b>771</b>
	<i>K.S. Thygesen and A. Rubio</i>	
23.1	Introduction	771
23.2	Formalism	773
23.3	Many-body self-energy	781
23.4	Current formula and charge conservation	786
23.5	Two-level model	791
23.6	Applications to C <sub>6</sub> H <sub>6</sub> and H <sub>2</sub> molecular junctions	802
23.7	Summary and perspectives	809
	Acknowledgments	810
	Appendix	810
	References	811
<b>24</b>	<b>Spin currents in semiconductor nanostructures: A non-equilibrium Green-function approach</b>	<b>814</b>
	<i>Branislav K. Nikolić, Liviu P. Zârbo, and Satofumi Souma</i>	
24.1	Introduction	814
24.2	What is pure spin current?	816
24.3	How can pure spin currents be generated and detected?	817
24.4	What is the spin-Hall effect?	817
24.5	What is the mesoscopic spin-Hall effect?	819
24.6	SO couplings in low-dimensional semiconductors	821
24.7	Spin-current operator, spin density, and spin accumulation in the presence of intrinsic SO couplings	833
24.8	NEGF approach to spin transport in multiterminal SO-coupled nanostructures	835
24.9	Computational algorithms for real $\otimes$ spin space NEGFs in multiterminal devices	853
24.10	Concluding remarks	860
	Acknowledgments	861
	References	861

<b>25 Disorder-induced electron localization in molecular-based materials</b>	<b>866</b>
<i>Sven Stafström and Mikael Unge</i>	
25.1 Introduction	866
25.2 Methodology	871
25.3 Results and discussion	879
25.4 Summary	887
Acknowledgments	889
References	889
<b>Subject Index</b>	<b>893</b>