

Contents

Preface XIII

List of Contributors XV

- 1 Molecular Information Processing: from Single Molecules to Supramolecular Systems and Interfaces – from Algorithms to Devices – Editorial Introduction 1**
Evgeny Katz and Vera Bocharova
References 7

- 2 From Sensors to Molecular Logic: A Journey 11**
A. Prasanna de Silva
 - 2.1 Introduction 11
 - 2.2 Designing Luminescent Switching Systems 11
 - 2.3 Converting Sensing/Switching into Logic 13
 - 2.4 Generalizing Logic 15
 - 2.5 Expanding Logic 16
 - 2.6 Utilizing Logic 17
 - 2.7 Bringing in Physical Inputs 20
 - 2.8 Summary and Outlook 21Acknowledgments 21
References 21

- 3 Binary Logic with Synthetic Molecular and Supramolecular Species 25**
Monica Semeraro, Massimo Baroncini, and Alberto Credi
 - 3.1 Introduction 25
 - 3.1.1 Information Processing: Semiconductor Devices versus Biological Structures 25
 - 3.1.2 Toward Chemical Computers? 26
 - 3.2 Combinational Logic Gates and Circuits 27
 - 3.2.1 Basic Concepts 27
 - 3.2.2 Bidirectional Half Subtractor and Reversible Logic Device 28
 - 3.2.3 A Simple Unimolecular Multiplexer–Demultiplexer 32
 - 3.2.4 An Encoder/Decoder Based on Ruthenium Tris(bipyridine) 36

3.2.5	All-Optical Integrated Logic Operations Based on Communicating Molecular Switches	38
3.3	Sequential Logic Circuits	41
3.3.1	Basic Concepts	41
3.3.2	Memory Effect in Communicating Molecular Switches	42
3.3.3	A Molecular Keypad Lock	43
3.3.4	A Set–Reset Memory Device Based on a Copper Rotaxane	46
3.4	Summary and Outlook	48
	Acknowledgments	49
	References	49
4	Photonically Switched Molecular Logic Devices	53
	<i>Joakim Andréasson and Devens Gust</i>	
4.1	Introduction	53
4.2	Photochromic Molecules	54
4.3	Photonic Control of Energy and Electron Transfer Reactions	55
4.3.1	Energy Transfer	55
4.3.2	Electron Transfer	59
4.4	Boolean Logic Gates	61
4.5	Advanced Logic Functions	64
4.5.1	Half-Adders and Half-Subtractors	65
4.5.2	Multiplexers and Demultiplexers	68
4.5.3	Encoders and Decoders	69
4.5.4	Sequential Logic Devices	71
4.5.5	An All-Photonic Multifunctional Molecular Logic Device	75
4.6	Conclusion	75
	References	76
5	Engineering Luminescent Molecules with Sensing and Logic Capabilities	79
	<i>David C. Magri</i>	
5.1	Introduction	79
5.2	Engineering Luminescent Molecules	80
5.3	Logic Gates with the Same Modules in Different Arrangements	83
5.4	Consolidating AND Logic	84
5.5	“Lab-on-a-Molecule” Systems	87
5.6	Redox-Fluorescent Logic Gates	90
5.7	Summary and Perspectives	95
	References	96
6	Supramolecular Assemblies for Information Processing	99
	<i>Cátia Parente Carvalho and Uwe Pischel</i>	
6.1	Introduction	99
6.2	Recognition of Metal Ion Inputs by Crown Ethers	100
6.3	Hydrogen-Bonded Supramolecular Assemblies as Logic Devices	102

- 6.4 Molecular Logic Gates with [2]Pseudorotaxane- and [2]Rotaxane-Based Switches 103
- 6.5 Supramolecular Host-Guest Complexes with Cyclodextrins and Cucurbiturils 110
- 6.6 Summary 116
- Acknowledgments 117
- References 117

7 Hybrid Semiconducting Materials: New Perspectives for Molecular-Scale Information Processing 121

Sylvia Gawęda, Remigiusz Kowalik, Przemysław Kwolek, Wojciech Macyk, Justyna Mech, Marek Oszajca, Agnieszka Podborska, and Konrad Szaciłowski

- 7.1 Introduction 121
- 7.2 Synthesis of Semiconducting Thin Layers and Nanoparticles 122
 - 7.2.1 Microwave Synthesis of Nanoparticles 123
 - 7.2.2 Chemical Bath Deposition 124
 - 7.2.2.1 Sulfide Ion Precursors 124
 - 7.2.2.2 Commonly Used Ligand 124
 - 7.3 Electrochemical Deposition 125
 - 7.3.1 Nanoheterostructure Preparation 133
 - 7.3.2 Nanoparticles Directed Self-Assembly 135
- 7.4 Organic Semiconductors—toward Hybrid Organic/Inorganic Materials 136
 - 7.4.1 Self-Organization Motifs Exhibited by Acenes and Acene-Like Structures 137
 - 7.4.2 Applications of Acenes in Organic Electronic Devices 141
- 7.5 Mechanisms of Photocurrent Switching Phenomena 142
 - 7.5.1 Neat Semiconductor 143
 - 7.5.2 Composite Semiconductor Materials 144
 - 7.5.3 Semiconductor–Adsorbate Interactions 148
 - 7.5.4 Surface-Modified Semiconductor 152
 - 7.5.5 Optoelectronic Devices Based on Organic Molecules/Semiconductors 160
- 7.6 Digital Devices Based on PEPS Effect 161
- 7.7 Concluding Remarks 167
 - Acknowledgments 168
 - References 168

8 Toward Arithmetic Circuits in Subexcitable Chemical Media 175

Andrew Adamatzky, Ben De Lacy Costello, and Julian Holley

- 8.1 Awakening Gates in Chemical Media 175
- 8.2 Collision-Based Computing 176
- 8.3 Localizations in Subexcitable BZ Medium 176
- 8.4 BZ Vesicles 180

8.5	Interaction Between Wave Fragments	181
8.6	Universality and Polymorphism	183
8.7	Binary Adder	186
8.7.1	Sum	188
8.7.2	Carry Out	191
8.8	Regular and Irregular BZ Disc Networks	193
8.8.1	Elementary Logic Gates	194
8.8.2	Half Adder	198
8.9	Memory Cells with BZ Discs	201
8.10	Conclusion	204
	Acknowledgments	204
	References	205
9	High-Concentration Chemical Computing Techniques for Solving Hard-To-Solve Problems, and their Relation to Numerical Optimization, Neural Computing, Reasoning under Uncertainty, and Freedom of Choice	209
	<i>Vladik Kreinovich and Olac Fuentes</i>	
9.1	What are Hard-To-Solve Problems and Why Solving Even One of Them is Important	209
9.1.1	What is so Good About Being Able to Solve Hard-To-Solve Problems from Some Exotic Class?	209
9.1.2	In Many Applications Areas –In Particular in Chemistry –There are Many Well-Defined Complex Problems	210
9.1.3	In Principle, There Exist Algorithms for Solving These Problems	210
9.1.4	These Algorithms may Take Too Much Time to be Practical	210
9.1.5	Feasible and Unfeasible Algorithms: General Idea	210
9.1.6	Solving Equations of Chemical Kinetics: An Example of a Feasible Algorithm	211
9.1.7	Straightforward Solution of Schrödinger Equation: An Example of an Unfeasible Algorithm	212
9.1.8	Straightforward Approach to Protein Folding: Another Example of an Unfeasible Algorithm	213
9.1.9	Feasible and Unfeasible Algorithms: Toward a Formal Description	213
9.1.10	Maybe the Problem Itself is Hard to Solve?	213
9.1.11	What Is a Problem in the First Place?	213
9.1.12	What is a Problem: Mathematics	214
9.1.13	A Description of a General Problem	214
9.1.14	What About Other Activity Areas?	214
9.1.15	What is a Problem: Theoretical Physics	215
9.1.16	What is a Problem: Engineering	215
9.1.17	Class NP	215
9.1.18	Class P and the $P \stackrel{?}{=} NP$ Problem	215
9.1.19	Exhaustive Search: Why it is Possible and Why it is Not Feasible	216

9.1.20	Notion of NP-Complete Problems	216
9.1.21	Why Solving Even One NP-Complete (Hard-To-Solve) Problem is Very Important	216
9.1.22	Propositional Satisfiability: Historically the First NP-Complete Problem	217
9.1.23	What We Do	217
9.2	How Chemical Computing Can Solve a Hard-To-Solve Problem of Propositional Satisfiability	218
9.2.1	Chemical Computing: Main Idea	218
9.2.2	Why Propositional Satisfiability was Historically the First Problem for Which a Chemical Computing Scheme was Proposed	218
9.2.3	How to Apply Chemical Computing to Propositional Satisfiability: Matiyasevich's Original Idea	219
9.2.4	A Precise Description of Matiyasevich's Chemical Computer: First Example	219
9.2.5	A Precise Description of Matiyasevich's Chemical Computer: Second Example	221
9.2.6	A Precise Description of Matiyasevich's Chemical Computer: General Formula	221
9.2.7	A Simplified Version (Corresponding to Catalysis)	222
9.2.8	Simplified Equations: Example	223
9.2.9	Chemical Computations Implementing Matiyasevich's Idea Are Too Slow	223
9.2.10	Natural Idea: Let us Use High-Concentration Chemical Reactions Instead	223
9.2.11	Resulting Equations	224
9.2.12	Discrete-Time Version of These Equations Have Already Been Shown to be Successful in Solving the Propositional Satisfiability Problem	225
9.2.13	Conclusion	225
9.2.14	Auxiliary Result: How to Select the Parameter Δt	226
9.3	The Resulting Method for Solving Hard Problems is Related to Numerical Optimization, Neural Computing, Reasoning under Uncertainty, and Freedom of Choice	228
9.3.1	Relation to Optimization: Why it is Important	228
9.3.2	Relation to Optimization: Main Idea	229
9.3.3	Relation to Numerical Optimization: Conclusion	231
9.3.4	Relation to Numerical Optimization: What Do We Gain from It?	231
9.3.5	Relation to Neural Computing	231
9.3.6	Relation to Reasoning Under Uncertainty	232
9.3.7	Relation to Freedom of Choice	233
	Acknowledgments	234
	References	234

10	All Kinds of Behavior are Possible in Chemical Kinetics: A Theorem and its Potential Applications to Chemical Computing	237
	<i>Vladik Kreinovich</i>	
10.1	Introduction	237
10.1.1	Chemical Computing: A Brief Reminder	237
10.1.2	Chemical Computing: Remaining Theoretical Challenge	238
10.1.3	What We Do	238
10.2	Main Result	239
10.2.1	Chemical Kinetics Equations: A Brief Reminder	239
10.2.2	Chemical Kinetics Until Late 1950s	240
10.2.3	Belousov – Zhabotinsky Reaction and Further Discoveries	240
10.2.4	A Natural Hypothesis	240
10.2.5	Dynamical Systems	241
10.2.6	W.l.o.g., We Start at Time $t = 0$	241
10.2.7	Limited Time	241
10.2.8	Limited Values of x_i	242
10.2.9	Limited Accuracy	242
10.2.10	Need to Consider Auxiliary Chemical Substances	242
10.2.11	Discussion	244
10.2.12	Effect of External Noise	245
10.3	Proof	246
	Acknowledgments	256
	References	257
11	Kabbalistic–Leibnizian Automata for Simulating the Universe	259
	<i>Andrew Schumann</i>	
11.1	Introduction	259
11.2	Historical Background of Kabbalistic–Leibnizian Automata	259
11.3	Proof-Theoretic Cellular Automata	264
11.4	The Proof-Theoretic Cellular Automaton for Belousov–Zhabotinsky Reaction	268
11.5	The Proof-Theoretic Cellular Automaton for Dynamics of <i>Plasmodium</i> of <i>Physarum polycephalum</i>	271
11.6	Unconventional Computing as a Novel Paradigm in Natural Sciences	276
11.7	Conclusion	278
	Acknowledgments	278
	References	278
12	Approaches to Control of Noise in Chemical and Biochemical Information and Signal Processing	281
	<i>Vladimir Privman</i>	
12.1	Introduction	281
12.2	From Chemical Information-Processing Gates to Networks	283
12.3	Noise Handling at the Gate Level and Beyond	286

12.4	Optimization of AND Gates	290
12.5	Networking of Gates	294
12.6	Conclusions and Challenges	296
	Acknowledgments	297
	References	297
13	Electrochemistry, Emergent Patterns, and Inorganic Intelligent Response	305
	<i>Saman Sadeghi and Michael Thompson</i>	
13.1	Introduction	305
13.2	Pattern Formation in Complex Systems	306
13.3	Intelligent Response and Pattern Formation	308
13.3.1	Self-Organization in Systems Removed from the Equilibrium State	309
13.3.2	Patterns in Nature	310
13.3.3	Functional Self-Organizing Systems	310
13.3.4	Emergent Patterns and Associative Memory	312
13.4	Artificial Cognitive Materials	314
13.5	An Intelligent Electrochemical Platform	315
13.6	From Chemistry to Brain Dynamics	321
13.6.1	Understanding the Brain	321
13.6.2	Brain Dynamics	323
13.6.3	Electrochemical Dynamics	324
13.6.4	Experimental Paradigm for Information Processing in Complex Systems	325
13.7	Final Remarks	327
	References	328
14	Electrode Interfaces Switchable by Physical and Chemical Signals Operating as a Platform for Information Processing	333
	<i>Evgeny Katz</i>	
14.1	Introduction	333
14.2	Light-Switchable Modified Electrodes Based on Photoisomerizable Materials	334
14.3	Magnetoswitchable Electrodes Utilizing Functionalized Magnetic Nanoparticles or Nanowires	336
14.4	Potential-Switchable Modified Electrodes Based on Electrochemical Transformations of Functional Interfaces	339
14.5	Chemically/Biochemically Switchable Electrodes and Their Coupling with Biomolecular Computing Systems	343
14.6	Summary and Outlook	350
	Acknowledgments	351
	References	352

15 **Conclusions and Perspectives** 355

Evgeny Katz

References 357

Index 359