

Table of contents

Deutsche Zusammenfassung.....	ii
Abstract.....	iv
Table of contents.....	vi
1 Introduction.....	1
1.1 Motivation.....	1
1.2 Numerical Simulation: State-of-the-art	5
1.3 Research Objectives.....	6
1.4 Thesis Outline	7
2 Fundamentals of Numerical Solar Cell Device Simulation	11
2.1 Introduction to Photovoltaic Energy Conversion	11
2.1.1 From Solar Radiation to Free Electron-Hole Pairs	11
2.1.2 Separation of Charge Carriers towards the Contacts	12
2.1.3 Extracted Current-Voltage Characteristics	14
2.2 Numerical Device Simulation	15
2.2.1 Setaurus Device	17
2.2.2 Quokka3	17
2.3 Optical Simulation	18
2.3.1 Geometrical Optics.....	18
2.3.2 Transfer Matrix Method for Thin-Film Layers.....	19
2.3.3 Band-to-Band Absorption.....	21
2.3.4 Free Carrier Absorption.....	22
2.3.5 Phong Illumination Model.....	24
2.4 Electrical Simulation of Semiconductors	25
2.4.1 Charge Carrier Statistics.....	25
2.4.2 Recombination of Charge Carriers	26
2.4.3 Semiconductor Equations and Charge Carrier Transport	29
2.5 Contact Formation and Advanced Contact Schemes	30
2.5.1 Definition and Fundamental Prerequisites of Contacts.....	30
2.5.2 Metal-Semiconductor Contacts	33
2.5.3 Fermi-Level Pinning.....	35
2.5.4 Traditional Doped Homojunctions	37
2.5.5 Passivating and Carrier-Selective Contacts	38
2.6 Tunneling through Energetic Barriers.....	39
2.6.1 Overview	39
2.6.2 Barrier Tunneling	41
2.6.3 Band-to-Band Tunneling (B2B)	43

2.6.4	Trap-assisted Tunneling (TAT).....	44
2.7	Material Properties.....	46
2.7.1	Amorphous Silicon.....	46
2.7.2	Transition Metal Oxides.....	47
3	Requirements for Efficient Hole Extraction in TMO-based SHJ Solar Cells	49
3.1	Abstract.....	50
3.2	Introduction	50
3.2.1	Motivation.....	50
3.2.2	Approach and Simulation Model.....	51
3.3	Design Rules for Hole-Selective TMO-based Contacts.....	53
3.3.1	Hole Extraction at the Induced c-Si Junction	53
3.3.2	Hole Extraction at the TMO/a-Si Junction	55
3.4	Signatures of Contacts with Non-Ideal Selectivity	57
3.4.1	S-shaped JV_{light} Curves.....	57
3.4.2	Temperature Dependence.....	59
3.4.3	Sun V_{oc} : Injection Dependence.....	60
3.5	Comparison with Experimental Results.....	61
3.5.1	Impact of the Fabrication Conditions for a-Si:H and MoO_x	61
3.5.2	Selectivity Issues with Post-Deposition Annealing of Evaporated MoO_x	63
3.6	Summary.....	63
3.7	Acknowledgments	64
3.8	Critical Discussion and Additional Information	64
4	Interfacial Oxides at TCO/Si Thin Films on the Carrier Transport of Passivating Contacts	67
4.1	Abstract.....	68
4.2	Introduction	68
4.3	Simulation Method	69
4.4	Results	71
4.4.1	Contact Resistivity Measurements for SHJ	71
4.4.2	Approach: Improved WF Matching by TCO Interlayers.....	73
4.4.3	FF Losses due to Insufficient Tunneling Transport.....	75
4.4.4	Possible Parasitic Interfacial Oxides on n-TOPCon	79
4.5	Conclusion.....	82
4.6	Acknowledgments	82
4.7	Appendix	83
4.8	Critical Discussion and Additional Information	84

5	Efficiency Roadmap for Evolutionary Upgrades of PERC Solar Cells by TOPCon	87
5.1	Abstract.....	88
5.2	Introduction.....	88
5.3	Simulation Method.....	89
5.4	Verification of Optical Model.....	91
5.5	Efficiency Roadmap for TOPCon on PERC	92
5.5.1	Influence of Electrical Gains and Optical Losses on the Maximum Power Output	92
5.5.2	Electrical Loss Analysis	95
5.5.3	Optical Loss Analysis.....	96
5.5.4	Influence of the Illumination Spectrum	97
5.6	Outlook: Influence of Future PERC Improvements	99
5.7	Conclusion	100
5.8	Acknowledgment.....	101
5.9	Appendix.....	101
5.10	Critical Discussion and Additional Information.....	103
6	The Race for the Best Silicon Bottom Cell: Efficiency and Cost Evaluation of Pero-Si Tandem.....	107
6.1	Abstract.....	108
6.2	Introduction.....	108
6.3	Approach and Modelling	109
6.3.1	Investigated Bottom Cell Concepts	109
6.3.2	Optical Model and Experimental Validation	112
6.3.3	Electrical Model	115
6.3.4	Cost Evaluation Model.....	116
6.4	Efficiency and Cost Evaluation.....	117
6.4.1	Analysis of Optical Losses	117
6.4.2	Electrical Analysis of the Bottom Cells.....	119
6.4.3	Cell and Module Production Cost Analysis.....	122
6.4.4	LCOE evaluation.....	125
6.5	Conclusion	127
6.6	Acknowledgements.....	129
6.7	Appendix.....	129
6.8	Critical Discussion and Additional Information.....	134
7	How to Make PERC Suitable for Pero-Si Tandem: A Simulation Study	139
7.1	Abstract.....	140

7.2	Introduction	140
7.3	Modeling Approach and Simulation Inputs	142
7.4	Results	145
7.4.1	Analysis of Optical Properties.....	145
7.4.2	Evaluation of full area (P[E]RC) versus locally contacted (sPERC) bottom cells	147
7.4.3	Evaluation of full area contacted PERC-like bottom cells	151
7.5	Overview of the Different PERC Front-Side Concepts	155
7.6	Conclusion	157
7.7	Acknowledgements.....	158
7.8	Appendix	159
7.9	Critical Discussion and Additional Information	162
8	Optimized Front TCO and Metal Grid Electrode for Pero-Si Tandem	163
8.1	Abstract.....	164
8.2	Introduction	164
8.3	Experimental Background and Modelling Approach.....	166
8.4	Optimization of the Front TCO Electrode	168
8.4.1	Analysis of Optical Losses	168
8.4.2	Analysis of Electrical Losses	170
8.5	Finger Metallization and Interconnection Concept.....	172
8.6	Cost Analysis.....	174
8.7	Conclusion.....	176
8.8	Acknowledgements.....	177
8.9	Appendix	177
8.10	Critical Discussion and Additional Information	179
9	Conclusion and Outlook	181
10	Appendix.....	187
	List of Abbreviations	187
	List of Symbols	190
11	List of Publications.....	192
	Peer-Reviewed Journal Publications	192
	Co-Authored Contributions to Peer-Reviewed Journal Publications	193
	Contributions to Conferences.....	194
	Co-Authored Contributions to Conferences	195
	Awards	195
12	Bibliography	196
	Danksagungen	221