Comprehensive Characterization and Modelling of Operation Mechanisms in Third Generation Solar Cells

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Martin T. Neukom

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Universität Augsburg University

Zürcher Hochschule für Angewandte Wissenschaften
School of Engineering
ICP Institute of Computational Physics

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1. Gutachter: Prof. Dr. Wolfgang Brütting
2. Gutachter: Prof. Dr. Armin Reller
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Abstract

Solar energy is one of the key enabling technologies for the transition to a zero-carbon society – a necessity to mitigate global climate change. Emerging photovoltaic technologies based on novel semiconductor materials offer new disruptive applications since they can be made light-weight, flexible and in arbitrary shape and colour. In so-called tandem structures novel materials like perovskite furthermore have the **potential to overcome the efficiency limits** of silicon solar cells. The first generation of solar materials was crystalline silicon. The second generation were inorganic thin-film solar cells. The emerging photovoltaic technologies studied in this thesis are therefore called **third generation solar cells**.

This thesis is **focused on understanding the physics** underlying third generation photovoltaics. The understanding of the physical processes and the quantification of loss mechanisms are crucial to improve the power conversion efficiency and the lifetime of these devices.

To gain insight into the physical processes measurement results from a variety of experimental characterization methods are compared with results from numerical solar cell simulation. The characterization methods consist of various optical and electrical measurements on solar cells in **steady-state, transient and frequency domain**. The developed simulation software solves the coupled differential equations describing charge transport by drift-diffusion as well as charge recombination in semiconductors.

Whereas other simulation studies have focussed on individual measurement techniques, this thesis presents a physical model and resulting **simulation data that reproduces the full variety of measurements with one set of parameters**. This approach allows a more accurate extraction of material parameters and a deeper insight into the physical processes of these solar cells. Such a comprehensive study is applied to an organic and a perovskite solar cell, both belonging to the category of third generation solar cells.

Additionally, a broad overview of solar cell characterization techniques and their interpretation is presented. For that purpose, various characterization techniques are simulated with systematically varied device and material parameters for a sample solar cell. The systematic simulation results provide a **guide for the interpretation of observed experimental results**.

In perovskite solar cells a hysteresis is often observed between the forward and reverse current-voltage scans. The simulation model can reproduce this behaviour and provide an explanation why this hysteresis is often dependent on the interface materials on both sides of the perovskite layer. This study further explains **why highly efficient solar cells often show less hysteresis**.

Finally, it is shown that only the **consideration of mobile ionic charges in conjunction with electronic charges** in the semiconductor drift-diffusion model allows to explain transient and frequency domain data of planar perovskite solar cells. A novel step response technique illustrates that the retraction of ionic charges from layer interfaces enables charge transport.