Beyond Conventional Solar Cell Device Simulations

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Abstract

Solar cell device simulations are a very convenient tool to support experimental research activities, whose major goal is to develop novel and more efficient types of solar cells. Key to the successful use of solar cell simulations are one-dimensional numerical solutions of the Poisson equation and the transport equations for electrons and holes under suitable boundary conditions [1]. Another very important aspect are suitable parameter sets, which simulate the quality of a real fabricated device and describe the optical, transport and electronic properties of bulk materials acting as absorber layers, transport layers and contacts.

A typical solar cell device simulation can be carried out with low numerical efforts, which seems to invite many users to simply mass produce solar cell simulations of rather modest quality. This leads to contradicting results and empty claims, which cannot really be reproduced in a real working device. Some of the major issues for these failed simulations are:

A) Purely hypothetical combinations of layers, which are incompatible in practice due to lattice mismatches, or simply due to chemical reactions among different layers.
B) Unrealisitc sets of simulation parameters, which are either inconsistent, outdated or sometimes simply irreproducible. Thus, any logical relation between simulated and real devices simply breaks down at one point.
C) Fundamental issues of light-matter interactions, which are often key to the efficiency of certain types of solar cells, cannot be covered by guesswork or by oversimplistic modelling of simulation parameters.

With our presentation, we will suggest several ways to improve the quality of solar cell device simulations. First of all, simulations should only be taken seriously, when credible experimental studies are also available for a given system. Only then can a systematic and detailed scientific analysis of a given system be carried out, and otherwise not.

Second, for rather novel types of devices, the existing numerical tools or parameter sets are often insufficient. In such a situation, the best option is to use analytical approaches [2], which use the same parameter sets and cover similar ground. We will discuss the underlying theory of these analytical approaches and give some examples.

Third, we will show that clean and consistent parameter sets can be obtained from first principles using density functional theory [3]. Using this approach, many fundamental aspects of charge carries transport and light-matter interactions can be included into advanced solar cell device simulations. We will discuss some examples from our own work in this field.

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