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Modelling and simulation of charge transport in perovskite solar cells

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Perovskite solar cells (PSCs) have become one of the fastest growing photovoltaic technologies within the last few years, for example perovskite/silicon tandem cells have become more efficient than single junction silicon solar cells [1]. However, which exact physical operation mechanisms play a fundamental role within such devices is not fully understood yet. Experiments indicate that on the one hand besides the movement of electric carriers, ion movement within the perovskite and on the other hand surface effects need to be taken into account. For this reason it is paramount to understand the electronic-ionic charge transport and the effects at inner interfaces within PSCs better via improved modelling and simulation.
In our contribution, we present a new drift-diffusion model for the charge transport in PSCs based on fundamental principles of thermodynamics and statistical physics [2]. Further, we introduce a finite volume based solver and corresponding simulations to underline the importance of our modelling approach.

1] A. Al-Ashouri et al., Monolithic perovskite/silicon tandem solar cell with >29% efficiency by enhanced hole extraction, Science 370 (6522) (2020), 1300–1309.
[2] D. Abdel, P. Vágner, J. Führmann and P. Farrell. Modelling charge transport in perovskite solar cells: Potential-based and limiting ion depletion, Electrochimica Acta 390 (2021).

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