NEGF theory of photovoltaics at the nanoscale - from quantum fields to solar cell characteristics

Urs Aeberhard

Abstract:
The last two decades have seen the emergence of a number of novel photovoltaic device concepts aiming at a solar energy conversion efficiency beyond the limitations of conventional bulk semiconductor single junction technologies. The implementation of such concepts, like the solar cells based on intermediate bands, hot carriers or multiple-exciton generation, are largely based on the exploitation of the peculiar and tunable optoelectronic properties of nanostructure device components. The resulting deviation from the bulk-like behaviour conventionally assumed in the description of photovoltaic devices prevents the use of the standard semiclassical theory for the investigation and simulation-guided optimization of such solar cell architectures. In this talk, an innovative and comprehensive framework for the theoretical description of nanostructure based solar cells is presented, which relies on a non-equilibrium quantum statistical mechanics formulation of the photovoltaic processes in open quantum systems. It corresponds to a combination of the Keldysh - or non-equilibrium Green's function - formalisms in the fields of inelastic steady-state quantum transport and quantum optics. After an outline of the general theory framework, applications thereof to the simulation of a variety of nanostructure based photovoltaic devices are discussed, with focus on quantum well architectures.

References:
U. Aeberhard, "Simulation of nanostructure-based and ultra-thin film solar cell devices beyond the classical picture", Journal of Photonics for Energy 4, 042099 (2014)

U. Aeberhard, "Theory and simulation of quantum photovoltaic devices based on the non-equilibrium Green's function formalism", Journal of Computational Electronics 10, 394 (2011)