

Institut für Physik **Physikalisches Kolloquium**



Donnerstag, 09.11.2023, 15:30 Uhr

Ort: Reichenhainer Str. 90; Zentrales Hörsaal- und Seminargebäude, Raum C10.013

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Machine learning and device modeling as an automated diagnostic tool for high-throughput research

Device modeling is extensively used in solar cell research going from simple models such as the Shockley diode equation or partial differential equations (PDE) to more complex models like Monte-Carlo or drift-diffusion (DD). These models are often used as a diagnostic tool to understand and quantify the main losses for a given device by reproducing experimental measurements.

However, one of the main criticisms about using complex models as a means to quantify material properties is the many fitting (10 to 40) parameters that need to be estimated. Many argue that with so many fitting parameters one could fit almost any model to the experimental data.

In this presentation, the challenges of using high-dimensional physical models to quantify material properties accurately will be addressed. As well as, how machine learning methods such as Bayesian optimization (BO) combined with high-throughput (HT) experimental data can be leveraged to study material properties at scale.

The potential of using modeling, BO and HT data will be illustrated by several case studies using different physical models (PDE or DD) and experimental methods such as (i) transient absorption spectroscopy, (ii) transient photoluminescence and microwave conductivity, (iii) light-intensity-dependent current-voltage characteristics.

The open-source package BOAR (Bayesian Optimization for Automated Research) will be introduced here as a flexible package to address many challenges of solar cell research such as smart experimental planning or fitting of high-dimensional models to experimental data. This package combined with PDE solvers and open-source DD package SIMsalabim provides an easy-to-use and flexible toolbox for solar cell research.



Alle Zuhörer sind ab 15:15 Uhr zum Kaffee vor dem Hörsaal eingeladen.

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