A COMSOL Multiphysics Approach To Simulate Graphene Defect Effect On Perovskite Solar Cells

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Abstract

Perovskite solar cells (PSCs) are a promising photovoltaic technology but their performance remains limited by incomplete absorption of incident photons, primarily due to reflection at the transparent front electrode [1]. To address this issue, interface engineering with graphene-based nanomaterials is explored as a route to improve light harvesting. While graphene has emerged as a promising transparent electrode due to its exceptional electrical and optical properties, its real-world performance is often affected by structural and chemical imperfections introduced during synthesis, growth/deposition, and transfer phase. Understanding how such defects can influence light absorption in PSCs is essential for the reliable integration of graphene in next-generation photovoltaic devices.

This work aims to investigate the impact of graphene defects and imperfectness on the optical absorption performance of perovskite solar cells (PSCs) using COMSOL Multiphysics®. In particular, in this study a 3D model of a multilayer perovskite solar cell stack (glass/ITO/TiO_2/$MAPbI_3$/MoO_3/Ag) is analyzed in frequency domain using the Wave Optics Module of COMSOL Multiphysics®. Periodic boundary conditions are applied at the lateral edges to represent an infinite periodic structure. Graphene is incorporated as a surface current density boundary condition at the interface between ITO and TiO_2. This approach follows the methodology outlined in [2], which details the finite element modelling of 2D materials like graphene in numerical simulations. Moreover, the refractive index and extinction coefficient of each layer in the solar cell stack derived from the COMSOL Material Library are taken into account. The model is calibrated to reproduce the absorptance profile of a reference PSC without graphene. The next phase involves modifying the surface conductivity parameters of the graphene layer to account for different levels of imperfection, including variations in chemical potential to simulate realistic scenarios of nonideal graphene layers. The results obtained confirm the baseline absorptance profile of a traditional PSC. The ongoing simulations aim to quantify how the presence of a defective graphene layer alters this optical response. By sweeping the conductivity values, the model is able to reveal performance thresholds and tolerances for graphene quality in practical device settings.

This study contributes to the advancement of knowledge in the application of 2D materials in photovoltaics, particularly by offering a modelling strategy to include graphene imperfections. The findings are expected to guide material scientists and device engineers in setting performance targets for graphene-based electrodes in PSCs, thereby aiding in the development of more efficient and reliable solar energy technologies.

Reference

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