Plasmonic Solar Cells: A Bridge between Electromagnetics and Semiconductor Physics

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A multiphysics study carries out on plasmonic organic solar cells (OSCs) by solving Maxwell's equations and semiconductor (Poisson, drift-diffusion, and continuity) equations simultaneously with unified finite-difference framework. (See *Applied Physics Letters*, 101, 223302, 2012; and *Optics Express*, 20, 2572-2580, 2012.) Regarding the Maxwell's equations, the perfectly matched layer and periodic boundary conditions are imposed at the vertical and lateral directions of OSCs to simulate the infinite air region and metallic grating electrode, respectively. In view of the semiconductor equations, the Scharfetter-Gummel scheme and semi-implicit strategy are adopted respectively in the space and time domains. To model the bulk heterojunction OSCs, the Langevin bimolecular recombination and Onsager-Braun exciton dissociation models are fully taken into account. The exciton generation rate depending on the optical absorption of the organic active material can be obtained by solving the Maxwell's equations and will be inserted into the semiconductor equations. Through the exciton generation rate, we seamlessly connect the optical with the electrical properties of plasmonic OSCs.

By introducing the metallic rectangular grating as the anode, surface plasmon resonances are excited resulting in extremely nonuniform exciton generation. Meanwhile, the built-in potential and internal electrostatic field of the plasmonic OSC device are significantly modified due to the modulated anode boundaries. From the theoretical model, we demonstrate that the plasmonic OSC structure improves 13% of short-circuit current but reduces 7% of fill factor compared to the standard one with a planar anode layer. The uneven photocarrier generation and transport induced by the metallic grating anode are the physical origins of the dropped fill factor. The spatially nonuniform exciton generation and internal electrostatic field distribution that strongly depend respectively on the optical and electrical responses of the metallic grating should be considered for the future design of plasmonic OSCs. This work provides fundamental multiphysics modeling and understanding for plasmonic organic photovoltaics.