Quantum approach to modelling of plasmon photovoltaic effect

Katarzyna Kluczyk[1], Christin David[2], Zofia Krzemińska[1], Witold A. Jacak[1]

[1]*Department of Quantum Technologies, Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology, Wybrzeże St. Wyspiańskiego 27, 50-370 Wrocław*

[2] *Department of Photonic Engineering, DTU, Denmark*

One of the crucial parameters affecting the solar cell efficiency is the absorption rate of the solar spectrum impinging on their surface. Metallic nano-particles (MNPs) where showed to improve this process – especially in a thin-film solar cells as the plasmon supported absorbing layer is of a few micrometer thickness – and ever since are of interest in various studies

Till today, three main mechanisms explaining the absorption enhancement in presence of MNPs were proposed: 1) the effective scattering of incident solar light on MNPs causing increase of the optical path length inside active layer and local enhancement of the electric field; 2) near field coupling between plasmon and semiconductor; 3) the direct generation of electron-hole pairs in the semiconductor.

While the observed scattering and field enhancement effects can be described with classical electrodynamic theory for most applications, the coupling between plasmons excited inside metallic nano-structures and semiconductor states in the solar cell can be only captured within quantum mechanics.

Within this paper we took the challenge to develop fast and reliable method for calculation of device optical properties while taking quantum effects into account. The idea was to modify the dielectric function of semiconductor substrate and MNP in such way to include the coupling between excited plasmons and semiconductor states. In the previous work we have applied the Fermi Golden Rule to calculate the probability of photon absorption with presence of spherical MNPs and compare it to the absorption without the MNPs [1]. Here we incorporate those formulas into numerical calculations within Finite Element Method (COMSOL). The first results suggests that the efficiency of energy transfer via near field coupling is much more effective than the absorption increase due to scattering on MNP. Interestingly even the parasitic absorption, due to ohmic loss inside MNPs seems to be insignificant after taking this coupling into consideration.

In the paper we present the absorption efficiency enhancement rates, due to MNPs, calculated including: near field coupling, only scattering effects and compare them with experimental findings.

[1] W. A. Jacak, E. Popko, A. Henrykowski, E. Zielony, K. Gwóźdź, G. Luka, R. Pietruszka, B. Witkowski, L. Wachnicki, M. Godlewski, L-B. Chang and M-J. Jeng, Solar Energy Materials & Solar Cells **147**, 1-16 (2016).