

Model of Electric Charge Transfer in Semiconductor/Electrolyte Interface Based on Drift-Diffusion Equations

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Abstract. Due to the enormous growth of the world's population, the demand for energy is also dramatically increasing. Most energy is currently produced on the basis of fossil fuels. However, this production raises a number of issues that have prompted research into new renewable energy sources. Hydrogen may be a suitable alternative to fossil fuels. It can be obtained by electrolysis of water or, for example, by photocatalytic decomposition of water molecules using solar energy. Efficient electrochemical processes are intensively studied and require extensive material research. Suitable semiconductor materials should be chemically stable and the energy gap should exceed the water splitting potential of 1.23 V with significant band-to-band absorption of solar radiation. Photoelectrochemical water splitting cells use a solid-liquid interface for the separation of produced electrical charges. This semiconductor-electrolyte interface substantially determines the water-splitting efficiency and therefore it is in the centre of scientific research. Modelling of the charge transfer at the photoelectrochemical interface provide important information about the dynamics of absorption processes connected with the energy band structure in contact with the electrolyte. This information can be obtained only by the numerical simulation. Modelling of charge transfer processes cover problems of the photon absorption, charge generation, transport and recombination processes. In our work we study numerical models describing these charge processes. The dynamics of charge carriers in the semiconductor is determined by the drift-diffusion equations, containing information about the charge densities, energy band structure and is influenced by electron and hole recombination processes (Shockley-Read-Hall, Auger and radiative recombination). Conclusions of numerical simulations are correlated with results of performed electrochemical experiments and used in the study of photoelectrochemical cell properties.