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Monitoring Photo-excitation and Electron-Hole Separation in Photovoltaic Materials[1] YOSHIYUKI MIYAMOTO, NEC — Efficiency of photovoltaic phenomena is governed not only by optical transition but also by separation of excited electrons and holes. However, these two events are in a tradeoff relation. For example, increasing optical transition rate by confining carriers in a quantum dot sacrifices carrier mobility and thus lowers electron-hole separation rate. For optimizing an efficiency of photovoltaic phenomena, theoretical analysis which can simultaneously treat photo-excitation and electron- hole separation are needed, while a conventional theory can merely treat these two events individually. In this presentation, I will introduce an approach of using the time- dependent density functional theory (TDDFT) for treating real- time propagation of electrons [1] under illumination of light which is mimicked by an alternating electric field. Then, photo- induced electron-hole creation and subsequent separation in polar crystallographic direction of 3C-SiC [2] will be demonstrated. In this simulation, the numerical stability was checked by the energy conservation rule [3] throughout the TDDFT simulation.

[1] O. Sugino and Y. Miyamoto, PRB**59**, 2579 (1999); PRB **66**, 89901(E) (2002).
[2] Y. Miyamoto, *submitted*.
[3] Y. Miyamoto and H. Zhang, PRB**77**, 165123 (2008).

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Yoshiyuki Miyamoto
NEC

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