A Study of non-Si Photovoltaic Materials based on an Analysis of Structural Stability Aimed for a High Efficiency

Project Representative

Masao Ichikawa

Honda R&D Co.,Ltd.

Authors

Katsutoshi Nosaki[*1], Tadahiro Kubota[*1], Syogo Tejima[*2], Terumi Furuta[*1], Masao Ichikawa[*1], Hisashi Nakamura[*2]

＊1　Honda R&D Co.,Ltd.

＊2　Research Organization for Information Science and Technology (RIST)

Abstract

Clean power generation is recognized as a serious issue in the energy supply of the 21st century in the environmental background such as the CO_2 exhaust amount control, the dryness of the oil resource and the limited production of biofuel so on. The solar energy down over the earth is large with 1.77×10^{16}kW. It is thought that solar batteries occupy an important position in the future clean power production. In the present, the Si crystal solar battery system is superior to the other solar cells. There are however some difficulties such as the production cost and a theoretical photoelectric limit of Si. Thus, it is required to shift to other materials for realizing more adequate solar power system. In this research, a new and high-efficient solar system is considered with non-Si material.

Base on the first-principles models, large-scale simulations have been carried out, by using the Earth simulator, for evaluating the stability of atomic structure, electronic state, light absorption of the photoelectric material in the solar cell. We have adopted an advanced GW approximation model for the excited state, instead of DFT models suitable for the ground state only. This makes it possible for us to analyze the band gap related to the light absorption and evaluate some controlling factors for realizing photoelectric materials with high efficiency. The large-scale simulations with high resolution models would surpass the existing photocell technologies and accelerate to realize the highly efficient solar cell.

Keywords： clean power generation, solar cell, first-principles calculation, GW approximation