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

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**Abstract**

Global warning and abnormal weather caused by $CO_2$ exhaust have a serious influence on the environmental problem. Reducing $CO_2$ exhaust for environmental protection depends on development of alternative energy such as clean sources instead of fossil fuel.

It is thought that solar batteries occupy an important position in the future clean power production because the solar energy down over the earth is large with $1.77 \times 10^{16}$kW. In the present, the Si crystal solar battery system is widely used in comparison with the other solar cells. There are, however, some difficulties such as the high production cost and limited incident photoelectric conversion efficiency. Thus, it is required to shift to other materials for next-generation solar power system. In this research, we investigated a new high-efficient solar material with non-Si material. On the basis of the first principles models, large-scale simulations have been carried out by using the Earth simulator. Simulations can evaluate the stability of atomic structure, electronic state, light absorption of the photoelectric material in the solar cell. The DFT models are a well-known less-accurate method to predict the band gap related to the light absorption. We have adopted an advanced GW approximation model treating with many body problem and hybrid method including a few phenomenologically-based parameters in the excited state, instead of DFT models suitable for the ground state only. This makes it possible for us to analyze the band gap accurately and evaluate some controlling factors. The large-scale simulations with high resolution models would accelerate the development of the highly efficient solar cell material.

**Keywords:** clean power generation, solar cell, first principles calculation, GW approximation, Hybrid DFT