Modeling and Experimental Characterization for Silicon-based Low-Cost High-Efficiency Photovoltaic technology

Approach

Materials Preparation and Device Fabrication: Optimizing the synthesis and layer deposition procedure of self-assembled silicon-based nanostructures to fit into the PV application. In developing experimental devices, activities will include investigation of low sheet resistivity contacting layers and fabrication of p-i-n structure with the desired interface property.

Simulation and Modeling

***Ab-initio* modeling using the first-principles calculation techniques**

Hardware

The calculations will be performed by using the high performance computing system at the Research Center for Applied Sciences, Academia Sinica (see http://warp.rcas.sinica.edu.tw/). The facility, which is called warp system and kindly provided by Prof. Yia-Chung Chang, (Director of Research Center for Applied Sciences Academia Sinica), consists 48 nodes, with 2 Intel Xeon 5160 (Dual Cores) CPUs and 8-16 GB memory in each node, and a more than 3 TB disk array for data storage.

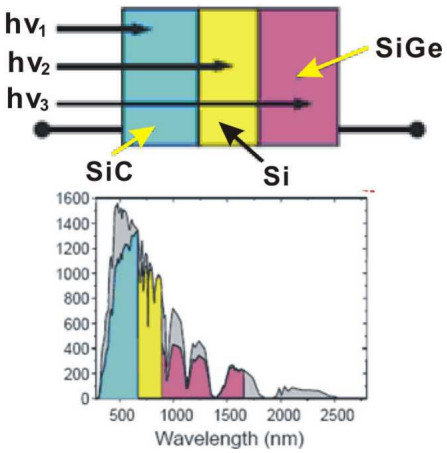
Software

The first-principles electronic structure calculation software LASTO (**L**inearized **A**ugmented **S**later-**T**ype **O**rbitial), developed by Prof. Yia-Chung Chang, is a highly efficient order-N package with a capability to handle complicated material system of hundred atoms per unit cell. The package had been installed and integrated into the web computing system. First-principles numerical modeling will be used to understand electronic structures of Si_xGe_{1-x}-Si-Si_yC_{1-y} thin-film system and Si quantum dots embedded in porous silica matrix, the resulting transport properties, and the effect of doping upon free carrier concentration.

The calculations to be completed are detailed as follows:

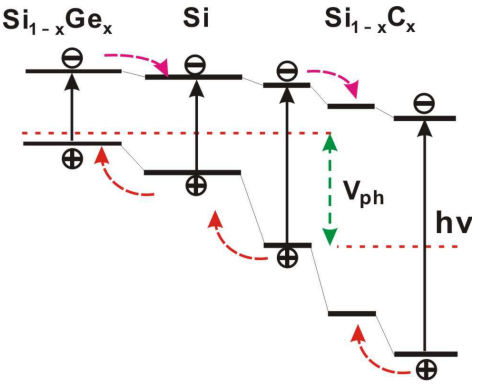
1st Year

Electronic structures of Si_xGe_{1-x}-Si-Si_yC_{1-y} thin-film system

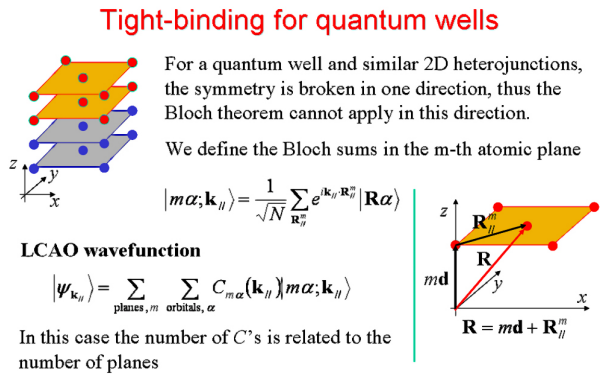


We shall improve the utilization efficiency of broadband solar photons in a PV device with a graded bandgap thin film system. This concept can be understood easily in the left diagram: If the heterostructure of a graded bandgap PV cell has a gradient of bandgap energy with reducing E_g from the front surface, an additional voltage arises owing to separation of the electrons and

the holes generated by photons of different energies in the different parts of the graded bandgap layer. However, to fully utilize this effect, new semiconductor materials with special properties should be developed. Low dimensional quantum well/dot structures open the room for preparation of such materials and PV cells.



Two material systems are to be investigated in this project. In the first year, we shall study the thin-film system of Si_xGe_{1-x}-Si-Si_yC_{1-y} theoretically. The operation principle of the PV effect in the thin film system is presented in the diagram on the left. The first-principles calculations of the electronic structures of Si_xGe_{1-x} and Si_yC_{1-y} with varying x and y will be conducted with LASTO in view of the efficiency of its algorithm. This calculation will yield a set of eigen-values and eigenfunctions of $\{\boldsymbol{E}_{nk}\}$ and $\{\boldsymbol{\Psi}_{nk}(\boldsymbol{r})\}$ for each alloy.



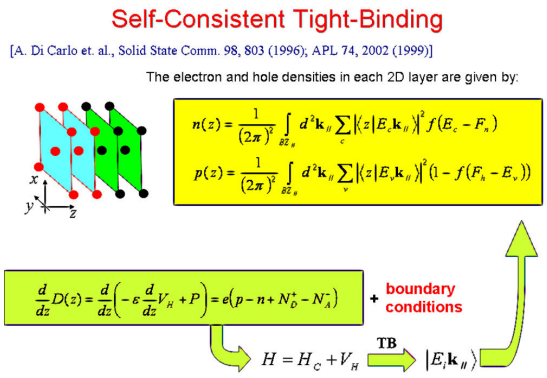
To model the cell heterostructure, $sp^3d^5s^*$ parameterization for tight binding (**TB**) Hamiltonian will be executed based on the results of LASTO calculation. This gives us merits of transferable and accurate interaction potentials and allows us to simulate large super cells, containing several hundreds of atoms. For 2D heterojunctions, the Density Functional Theory (DFT)-based TB procedure that we are going to implement is described briefly as follows: (1) First the Bloch sums with $\boldsymbol{k}_{||}$ in the m-th atomic plane are defined as

$|m\alpha;k_{||}\rangle = \frac{1}{\sqrt{N}}\sum_{R_{||}^m} e^{i\vec{k}_{||}\cdot\vec{R}_{||}^m}|R\alpha\rangle$ in terms of the α-orbital at the $\boldsymbol{R}$ position; (2) the wavefunctions determined from LASTO can then be rewritten as

$|\Psi_{k||}\rangle = \sum_{m\in planes}\sum_{\alpha\in orbitals} C_{m\alpha}(k_{||})|m\alpha;k_{||}\rangle$; (3) By using the wavefunctions, we can transform the Schrodinger equation into a matrix form of $\sum_{m=-M}^{m=+M} H_{l,l+m}C_{l+m} = EC_l$, where M is the number of interacting atomic planes and $\boldsymbol{H}$ is a very sparse matrix. By using the efficient calculation scheme, we plan to investigate the band alignment offsets at each interfaces of the Si_xGe_{1-x}-Si-Si_yC_{1-y} thin-film system with varying x and y. Global optimization may be executed to discover the best band structural profile for the PV application purpose.

2nd Year

Charge transport properties of Si_xGe_{1-x}-Si-Si_yC_{1-y} thin-film system



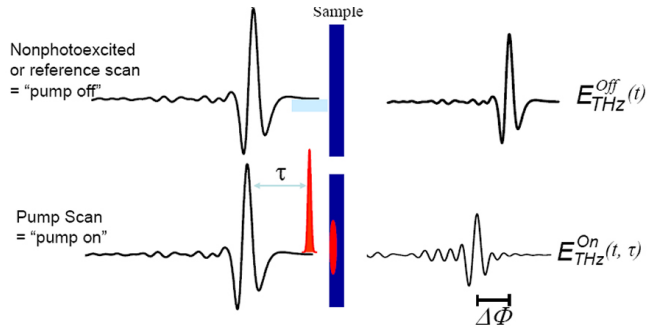
The self-consistent procedure can be implemented as depicted in the diagram on the left by integrating the TB procedure with Poisson equation to determine the built-in field that will be used to separate the photo-excited electrons from holes carriers.

3nrd Year

Impaction ionization and charge transport properties of silicon quantum-dots embedded in mesoporous silica

To increase the PV efficiency by producing a second or more electron-hole pair per absorbed photon through impact ionization requires that the rate of impact ionization is greater than the rate of carrier cooling and Auger processes. Although nanotechnology has considerable potential to separately tuning carrier transport and phonon dynamics to produce photovoltaic cells with significant increase in conversion efficiency, to fully realize the potential theoretical modeling is indispensable for giving an accurate guidance. We will perform the simulation on silicon quantum-dots embedded in mesoporous silica with DFT-based TB calculation developed in the previous years. In particular, impaction ionization and charge transport properties will be evaluated to either verify the functionality or tune the material structure for optimizing the PV effect.

Optical, and Electronic Characterization



$$\frac{\Delta E_{THz}(t,\tau)}{E_{THz}^{Off}(t)} \cong \frac{-\sigma(\tau)x}{2cn\varepsilon_o}$$

- Measure transient THz frequency average conductivity
- Subpicosecond resolution
- Mechanistic information
- No electrical contacts

The synthesis of high-quality materials must be coupled to the development and exploitation of new characterization tools capable of resolving elementary physical processes at appropriate length (x) and time scales (t) and with sufficient energy resolution (ν). We plan to detect multiexciton effect in silicon quantum dots in meso porous matrix and charge transport properties of Si_xGe_{1-x}-Si-Si_yC_{1-y} thin-film system with ultrafast spectroscopic method (such as femtosecond UV/visible-pump and THz-probe) to reveal photo-carrier distribution and

dynamic process. THz probing can be employed to map out transient free carrier density by adjusting the time delay as shown in the left diagram. By adjusting the pump wavelength, we can also probe the carrier dynamics starting at varying depth of Si_xGe_{1-x}-Si-Si_yC_{1-y}. This yields a glimpse of the transport dynamics of photo-excited carriers. If direct measurement of current generated by a solar cell is also conducted and combined with the information deduced from ultrafast spectroscopic method, a complete picture of PV effect in the material systems shall be yielded.