A Supercomputing Study of Photovoltaic Quantum Dots

Shanshan Wu^{1,2}, Michael McGuigan² James Glimm^{1,2}, James Davenport², Stan Wong^{1,2}, Amanda Tiano^{1,2}

1. Stony Brook University Brookbayen National Laborator

2. Brookhaven National Laboratory





Renewable Energy Share of Global Final Energy Consumption, 2008





-- Renewables 2010 Global Status Report

Growth Rates of Renewable Energy Capacity



Cost of Electricity by Source



ST NY BR K

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-- http://www.claverton-energy.com/?dl_id=385

Efficiency of Photovoltaic Solar Cell

Materials	Efficiency
Crystalline	12 – 40%
Thin film	7 – 10%
Quantum Dot	Up to 65%



-- Renewables 2010 Global Status Report

-- http://www.futurepundit.com/archives/002789.html

Quantum Dot Solar Cell

• Basic structure:

A quantum dot, composed of semiconducting material, placing on a silicon substrate.

• Active element:

The properties of quantum dot, especially its band gap, determine the efficiency of the solar cell.

ST MANected via organic linker to a drain, modeled as BR Solution

Molecule Visualization



CdSe dot and Gold dot are connected by sulfur atoms with linker.

-- Visualized by VMD



Comparison of Band Gaps





- -- DFT B3LYP exchange correlation potential
- ---Gaussian basis set, core potential, NWChem 5.0

Energy States Overlap Computation

• Fermi's Golden Rule

$$T_{i \to f} = \frac{2\pi}{\hbar} \left| \left\langle f \left| \vec{d} \right| i \right\rangle \right|^2 \rho$$

where P is the density of final states (number of states per unit of energy), and $\langle f | \vec{d} | i \rangle$ is the matrix element of the dipole moment \vec{d} between the final and initial states

$$\vec{d} = e\left(\sum_{i} x_{i}, \sum_{i} y_{i}, \sum_{i} z_{i}\right)$$

 Under the same grid system, the inner product of energy states could be approximated by multiplying the data of wave functions.



Band structure of CdSe18 and linker



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