innovation

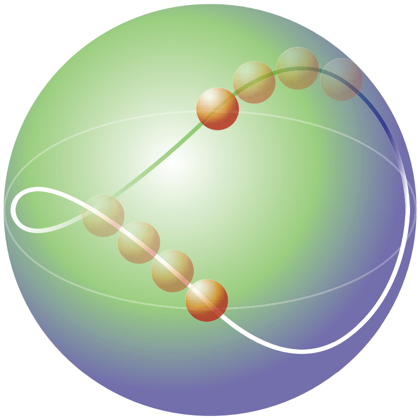
Quantum Dots Promise to Significantly Boost Photovoltaic Efficiencies

In the sometimes strange world of nanoscale materials, unexpected things can happen. This is exactly what scientists at the National Renewable Energy Laboratory (NREL) have discovered while exploring quantum dots (QDs). These semiconductor nanocrystals typically have diameters from about 2 to 10 nanometers (nm, or one billionth of a meter) and contain only hundreds to thousands of atoms. But they could do great things when it comes to generating electricity.

Semiconductor quantum dots used in so-called "third-generation" solar cells have the potential to dramatically increase—in some cases even double—the efficiency of converting sunlight to electricity. The conversion process works via "multiple exciton generation (MEG)." In this process, when a single photon of light of sufficient energy is absorbed by the quantum dot, it produces more than one bound electron-hole pair, or exciton. NREL scientists were the first to predict this important unusual MEG effect in QDs, which contrasts with conventional photovoltaic (PV) cells having much larger crystals and many more atoms and in which one photon produces only one electron-hole pair. The electronic process is also very fast, occurring within 200 femtoseconds—or 200 million billionths (10^{-15}) of a second.

MEG + Tuning = High Efficiency

Quantum dots exhibit other strange behavior in addition to multiple exciton generation. For example, varying the size of QDs can "tune" them to different wavelengths of light to optimize their performance. In essence, QDs can be tailored to absorb or emit specific wavelengths of light simply by changing the size of the dot . Compared with bulk materials, which have larger crystals and more atoms than nanomaterials, the light spectra emitted or absorbed by QDs will shift to the blue, which represents greater energy or shorter wavelength. Thus, the smaller the dot, the greater the shift.



For an electron to exist within a confined space—such as in a spherical quantum dot—it must have an associated wavelength equal to the inside circumference of the confining space or a whole number fraction thereof. The smaller the dot, the shorter the wavelength that fits and the higher the energy of the electron. Hence, the absorption and emission spectra shift to the blue (higher energy) for smaller dots. In essence, NREL scientists can tailor quantum dots to absorb or emit specific wavelengths of light simply by changing the size of the dot.

The Spectrum of
Clean Energy Innovation

- **Fundamental Science**
- Market-Relevant Research
- Systems Integration
- Testing and Validation
- Commercialization
- Deployment

Through deep technical expertise and an unmatched breadth of capabilities, NREL leads an integrated approach across the spectrum of renewable energy innovation. From scientific discovery to accelerating market deployment, NREL works in partnership with private industry to drive the transformation of our nation's energy systems.

This case study illustrates NREL's innovations in Fundamental Science.

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

Taking advantage of both these effects—multiple exciton generation and energy tuning due to size of the nanocrystals—QDs can be incorporated into unique third-generation solar cells. These cells may produce both electricity and solar fuels with potentially very high efficiencies. Using detailed thermodynamic calculations, NREL has shown that QD solar cells operating under concentrated sunlight can have maximum theoretical conversion efficiencies twice that achievable by conventional solar cells—up to 66%, exceeding the theoretical efficiency limits of about 31% of present-day first-generation (silicon) and second-generation (thin-film silicon, cadmium telluride, and copper indium gallium diselenide) solar cells.

Advancing to Silicon Quantum Dots

NREL makes quantum dots from various materials, including cadmium selenide, cadmium sulfide, cadmium telluride, indium phosphide, indium arsenide, lead selenide, and lead sulfide. NREL scientists were also the first to observe the MEG effect in silicon nanocrystals—a critical step toward practically implementing these new types of efficient solar cells based on the most important and prevalent solar cell material, silicon.

Efficient MEG in silicon QDs can occur with relatively large (10-nm-diameter) nanocrystals, which maintain the favorable characteristic of absorbing light in the visible spectrum. Calculations show that silicon QDs with this optimal characteristic have a theoretical conversion efficiency of 40%. This means that silicon nanocrystals can potentially be used in QD solar cells to produce much higher efficiencies and lower cost PV using an abundant, environmentally friendly material.

However, before technologically significant solar cells become a reality, scientists must learn how to split or dissociate the excitons and collect the resulting free electrons and holes with high efficiency. Therefore, NREL is pursuing a better understanding of the fundamental science of MEG processes to develop solar cells with predicted high efficiencies. NREL has produced quantum dots using colloidal suspensions (see sidebar); then, using molecular self-assembly, these QDs have been fabricated into first-ever devices that operate with 4% efficiency and demonstrate the capability for low-cost manufacturing.

And There's More…Singlet Fission

NREL is also studying a process known as singlet fission, which is an analogous MEG effect in molecular chromophores. These molecules, which are able to reflect wavelengths of light in the visible spectrum, can produce two triplet excited states for every singlet excited state produced by absorbing one photon. Each of the triplets then produces an electron-hole pair. This process represents a possible disruptive means to get beyond the 32% conversion efficiency limit for a dye-sensitized Graetzel cell to a theoretical 47% limit for a specially designed solar cell device. In collaboration with the University of Colorado and Northwestern University, NREL has shown that unique molecular chromophores—for example, 1,3-diphenylisobenzofuran—can be designed to optimize singlet fission and exhibit exciton multiplication.

The theoretical and experimental work in nanocrystals being done by NREL scientists opens the door to the potential application of multiple exciton generation to greatly enhance the conversion efficiency of solar cells based on silicon and other semiconductor materials. The result is that more of the sun's energy may be available to generate solar electricity and produce solar fuels. This is a key step toward making solar electricity and fuels more efficient and cost competitive with conventional power sources.

How NREL Grows Great Quantum Dots

NREL scientists use two different approaches to fabricate QDs, both of which can be self-organizing.

Epitaxial growth involves growing crystals of one semiconductor material on the surface of another, and the structural (or crystal lattice) orientation of both materials is the same. NREL researchers use the Stranski-Krastanow growth method, in which the mismatched geometry of crystal lattices produces strains between the two materials, thus causing "islands" to form. Most of the material deposited—by the vacuum techniques of either molecular-beam epitaxy or metal-organic chemical vapor deposition—accumulates on the islands, forming a matrix of QDs whose size can be controlled by growth conditions.

Colloidal chemistry, which is NREL's primary method of growing QDs, is inexpensive, requiring only the proper chemicals, low-cost equipment, and room-temperature processing. Colloids are ultra-fine particles suspended in a liquid solution. The formation of QDs involves a chemical reaction between a metal ion (such as indium) with a molecule that donates a different ion (such as phosphide). The size of a QD is manipulated by controlling the concentration of the reactants, the medium in which they react, the temperature of the reaction, and the duration of the reaction. One difficulty is keeping QDs from agglomerating when they have reached the desired size. Generally, this is done by having the reaction occur in the presence of organic molecules that act as surfactants and coat the surface of the nanoparticles.

NREL has produced 4%-efficient solar devices using quantum dots grown from colloidal suspensions followed by molecular self-assembly.

National Renewable Energy Laboratory

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