Novel Automated Designs and Rapid Multivariate Optimization of Next-Generation Multijunction Quantum Dot Solar Cells Using Monte Carlo Modeling

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Large-scale adoption of solar power is limited by high cost compared to fossil fuel-based power generation. Multijunction quantum dot solar cells offer a potential high-efficiency, low-cost solution. Despite high performance in quantum dot solar cells (QDSCs), lead sulfide quantum dots (QDs) have not been thoroughly studied in multijunction solar cells. To optimize multijunction QDSC efficiency by characterizing photon-quantum dot interactions, quantum mechanically cloud-computed absorption spectra of lead sulfide QDs of various diameters and the solar radiation spectrum on Earth's surface were incorporated into Java-programmed Monte Carlo simulations implementing novel algorithms. Algorithms were developed and executed to quantify photon absorption-electricity conversion synergy. After thousands of hours of computation, 6,132 multivariate simulations were conducted spanning design permutations for 1- to 9-junction QDSCs of constant solar cell thickness for various QD diameters and bandgap standard deviations. Solar spectral changes and optimal energy conversion efficiencies were tracked as photons passed through junctions. A program was written to automatically sort through the efficiency results, taking into consideration the thermodynamic model proposed by De Vos et al. Computed optimized efficiencies were 39.2%, 51.5%, 57.7%, 62.8%, 64.5%, 66.7%, 68.1%, 68.4%, and 68.7% for 1- to 9-junction QDSCs under concentrated sunlight, compared to the 33.7% Shockley-Queisser limit of conventional solar cells. This work constructed and demonstrated a novel methodology using computation to rapidly achieve optimal designs for multijunction QDSCs. Wider application of this technique could enable and significantly accelerate multijunction QDSC development and adoption.

Awards Won:

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