Designing Photonic Crystals in Strongly Absorbing Material for Applications in Solar Cells and Photosensors.

Minda Wagenmaker[1], Ebuka S. Arinze[2], Botong Qiu[2], Susanna M. Thon[2]

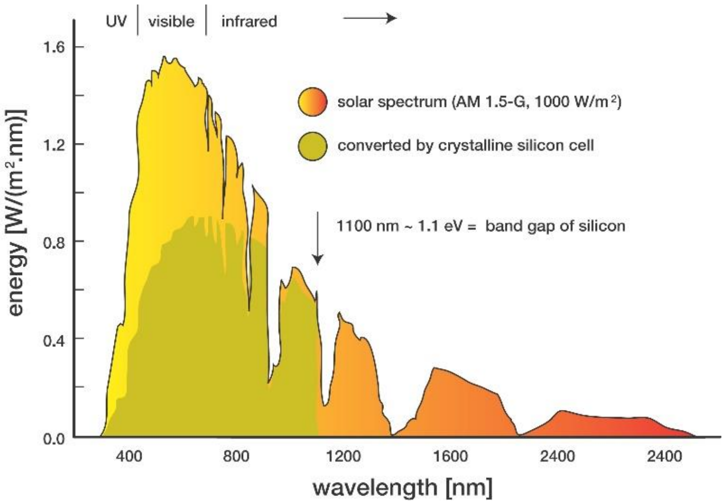
[1]Mechanical Engineering Department, The University of Alabama
[2]Electrical and Computer Engineering Department, Johns Hopkins University

Abstract

The solar industry, becoming cost competitive with natural gas, has proven to be a safer alternative in terms of protecting the environment. A potential way to make solar cells more efficient is by designing a wavelength selective material to expand the range of wavelengths a solar cell system can absorb and convert into electricity. Similarly, this material could be applied towards improving wavelength-selective photosensing in broadband semiconductors. This study has shown that the transmission of visible wavelengths through an infrared top cell (colloidal quantum dot film) can be increased by 115% via photonic crystals. This crystal structure has been optimized by incorporating 250 nm dielectric inclusions in a hexagonal arrangement within a 250 nm thick CQD film. Additionally, adding an antireflective coating composed of 140 nm thick aluminum-doped zinc oxide and 100 nm thick molybdenum trioxide, reduces average reflection between wavelengths 400-1200 nm by 19% to further enhance high transmission and absorption over the desired wavelength ranges.

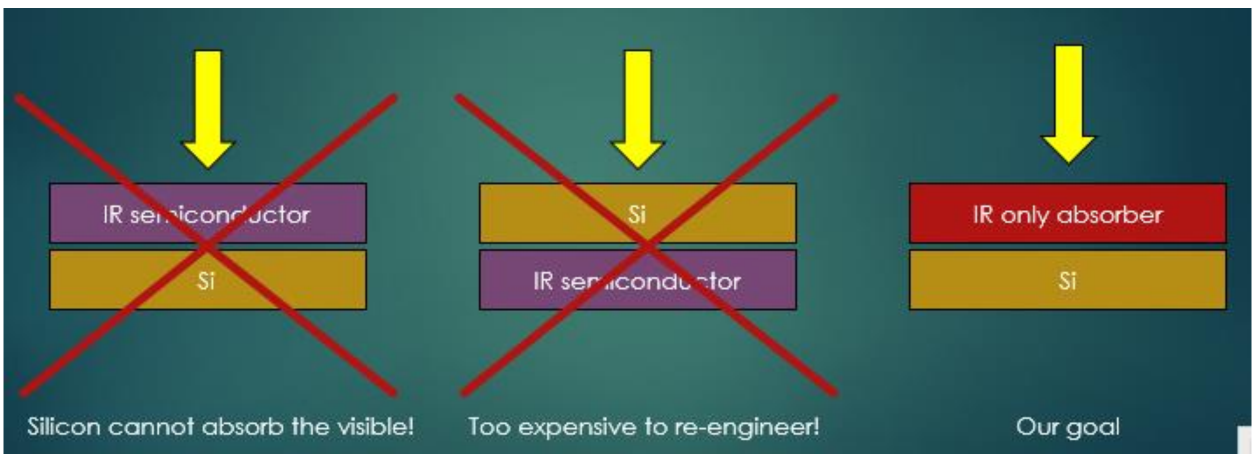
Background

Traditionally, silicon solar cells can only absorb the wavelengths smaller than their bandgap (located at 1100 nm), therefore most of the infrared wavelengths irradiated by the sun are unabsorbed and are lost potential. (See Figure 1)



(Fig. 1) Spectrum of the sun's solar radiation

By designing a tandem solar cell with a CQD-based solar cell on top of a silicon solar cell, we can increase the range absorbed by the sun and therefore increase the efficiency of solar cells.



(Fig. 2) Various tandem solar cell designs

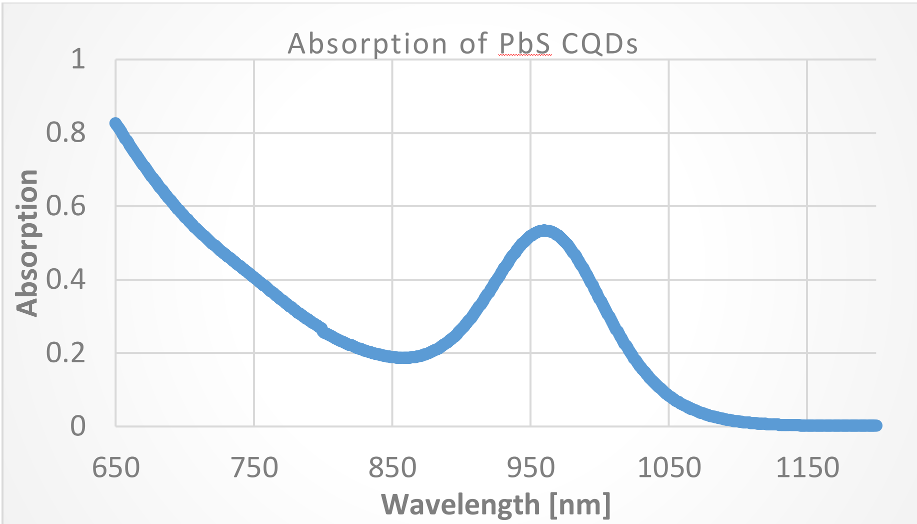
In tandem cell structure, there must be current matching between the CQD-based cell and the silicon solar cell layer. This means both layers need to absorb the same number of photons to generate the same current, as tandem solar cells generally work in series. Thus, it also needs to transmit some visible wavelengths otherwise the infrared cell will absorb everything and there will be no transmission to the cell below. Only then can we utilize the pre-existent manufacturing process and design for the silicon solar cell. This is a much cheaper alternative to re-engineering the tandem solar cell design and manufacturing process by switching the order of the solar cells. (See Figure 2)

Photonic Crystals

One potential route to achieve our goals is via photonic crystals. A photonic crystal is a periodic arrangement of alternating materials with different dielectric constants. It creates periodic potentials for light, providing bandgaps for photons in the same way semiconductors provide bandgaps for electrons. Although in the past photonic crystals have been observed to create bandgaps in dielectric or non—absorbing materials, in this study the objective is to apply photonic crystals and manipulate light in absorbing materials, namely colloidal quantum dots.

Colloidal Quantum Dots [CQDs]

Colloidal Quantum Dots are nanoscale semiconductive particles, suspended in solution. The size of the dots correlates to the size of their bandgap. We can manipulate the size of the dots, and therefore the optical properties of the quantum dot solution, by altering the injection temperature during synthesis. To synthesize lead sulfide (PbS) CQDs, a lead precursor must be prepared by stirring on high heat and under vacuum pressure for at least 16 hours. Next, the lead precursor is injected with a sulphur precursor at an appropriate temperature ranging from 90-120 °C. This temperature determines the size of the dots and therefore the absorption onset of the semiconducting material. An injection at 120 °C enables the first exciton peak to be located at 960 nm.



(Fig. 3) Absorption spectrum of CQDs synthesized in the lab

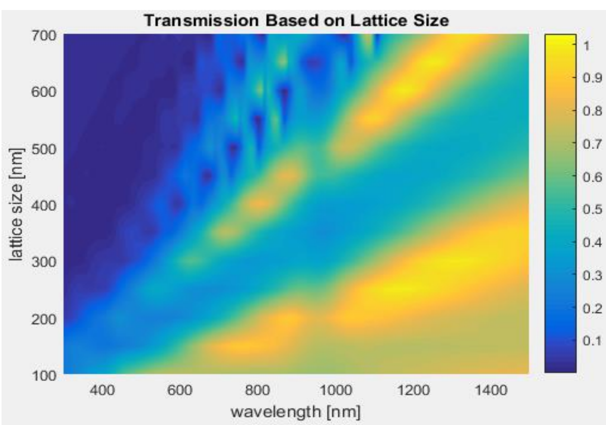
The benefits of using CQDs as the strongly absorbing material include their ability to absorb in the infrared, their controllable absorption peak, and the fact that they are solution processed, making them easier to integrate into solar cells or other optoelectronics.

Methods

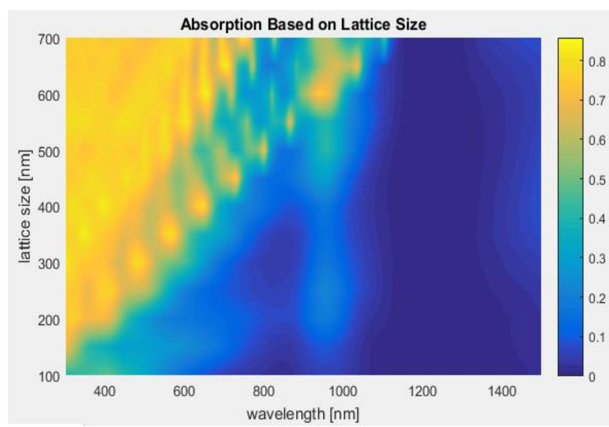
To determine the optimal system to achieve high absorption in the infrared and high transmission in the visible, using a CQD film and a dielectric material as the two alternating materials of the photonic crystal, Lumerical Finite Difference Time Domain [FDTD] Solutions was used. This software program solves coupled differential equations, which in this case were Maxwell's equations, on a discretized grid in time and space. After setting the grid size, time step, light source, material and structure of the model, the program outputs the electromagnetic field distribution, from which we the absorption, transmission, and reflection at each wavelength of light can be calculated. Various simulation parameters were tuned including the materials, inclusion size, inclusion spacing, film thickness, inclusion shape, and lattice arrangement to optimize the optical properties. Finally, an antireflective layer was designed to solve the in-coupling problem of the photonic crystal and trap photons from reflecting into the atmosphere thus enabling them to be absorbed or transmitted instead. Aluminum-doped zinc oxide and molybdenum trioxide were used as the antireflective coating, because not only do they have differing refractive indices, but they also serve a practical electronic use as a top contact for the solar cell.

<u>Results and Discussion</u>

The results from the Lumerical FDTD simulations assisted in the identification of system with a 250 nm sized inclusions within a 250 nm thick film with 250 nm spacing to have the best tradeoff with the highest transmission in the visible range [400-600 nm], while maintaining high absorption in the infrared range [800-1200 nm]. Based on the control of a pure CQD film, Fig. 1(a) shows this crystal has a 115% increase in visible transmission [from 13% to 18%] and Fig. 1(b) shows it only suffers a 19% infrared absorption loss [from 10% to 8%].

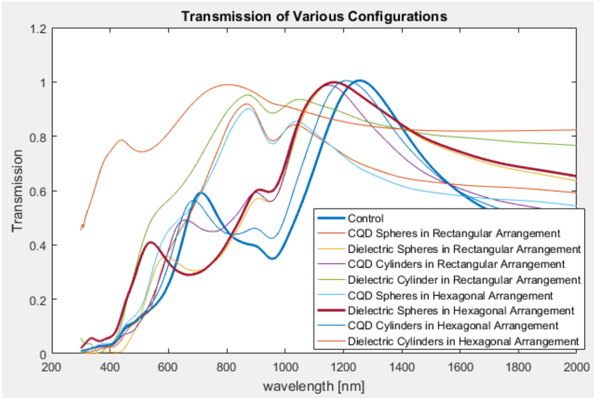


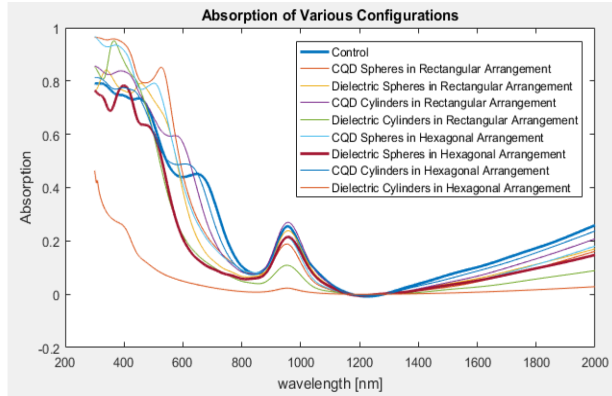
(Fig. 4 (a)) Transmission of the CQD-based cell as the film thickness, spacing, and inclusion diameter increase proportionally



(Fig. 4 (b)) Absorption of the CQD-based cell as the film thickness, spacing, and inclusion diameter increase proportionally

The hexagonal arrangement was identified to have the highest visible transmission (See Figure 4(a)) for still having comparable infrared absorption to the control (See Figure 4(b)).

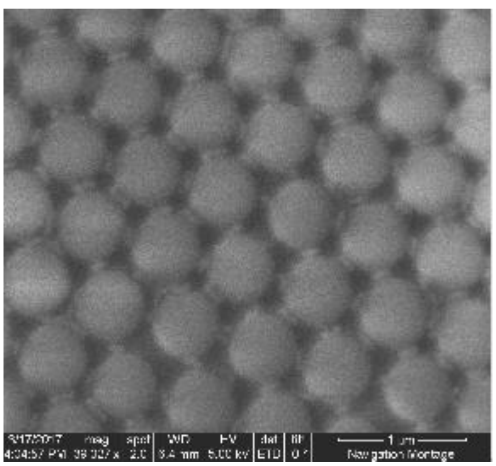




(Fig. 5 (a)) Transmission of the CQD-based cell with various inclusion shapes and material in hexagonal and rectangular arrangements

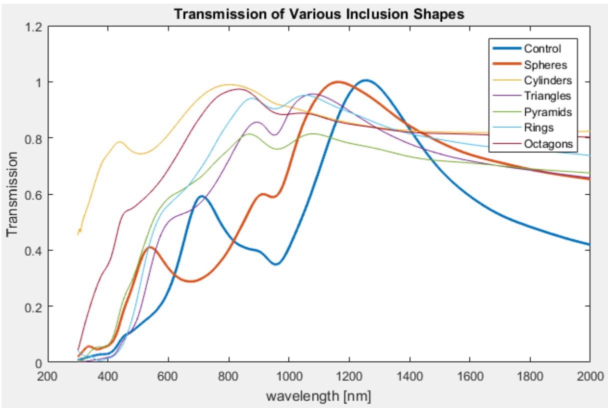
(Fig. 5 (b)) Absorption of the CQD-based cell with various inclusion shapes and material in hexagonal and rectangular arrangements

And another reason in favor of the hexagonal arrangement is ease of fabrication. Figure 5 below is of polystyrene beads spin coated onto a glass substrate in the lab. The beads naturally self-assemble into a hexagonal arrangement.

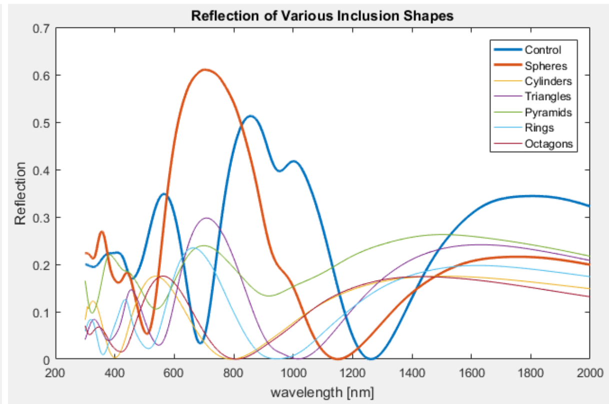


(Fig. 6) A Scanning Electron Microscope (SEM) image of polystyrene bead in hexagonal formation

The spherical inclusion shape is the most promising of them to work with. Figure 7(a) shows the transmission peak over the visible range, which is where peak transmission is desired. From that as a starting point, ways to increase that peak can be explored. Additionally, the fact that the transmission dips down in the infrared range, shows promise that the crystal might be absorbing there instead. However, if it's not absorbing, but is really reflecting, as shown in Figure 7(b), an antireflective coating can be applied to counter the reflection and encourage the light to reflect back into the CQD-based cell to be absorbed instead.

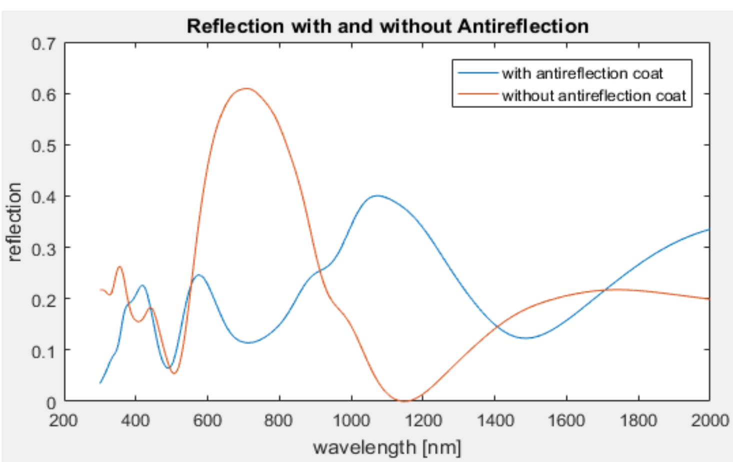


(Fig. 7 (a)) Transmission of the CQD-based cell with various inclusion shapes compared to the pure CQD film control



(Fig. 7 (b)) Reflection of the CQD-based cell with various inclusion shapes compared to the pure CQD film control

A designed antireflective coating of 140 nm of aluminum-doped zinc oxide [AZO] on top of 100 nm of molybdenum trioxide reduces average reflection over the range 400 nm – 1200 nm by 16% (See Figure 8).



(Fig. 8) Reflection of the CQD-based cell with 250 nm dielectric spherical inclusions within a 250 nm thick CQD film and a 140 nm AZO / 100 nm MoO_3 antireflective coating compared to the control of the 250 nm dielectric spherical inclusions within a 250 nm thick CQD film without any antireflective coatings.

Conclusion

The optimal photonic crystal structure we've identified is 250 nm dielectric spheres with 250 nm spacing within a 250 nm thick CQD film in a hexagonal arrangement. This designed system shows 115% higher visible transmission and only suffers a 19% infrared absorption loss. Future work in this study will include calculating full photonic band structures, to systematically work towards further increasing both visible transmission and infrared absorption, fabrication and testing of real structures and devices.