Project: “Nanostructured Silicon-Based Tandem Solar Cells”
Institution: University of New South Wales, Sydney, Australia

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Introduction
The aim of the project is the development of a potentially “game-changing” photovoltaic technology (today’s highest efficiencies at tomorrow’s lowest projected costs) by innovative exploitation of past silicon solar cell developments at the University of New South Wales (UNSW). The new technology combines low-cost polycrystalline silicon thin-films with higher bandgap material synthesized using silicon quantum dots in a matrix of silicon oxide, nitride, or carbide to produce 2- or 3-cell tandem stacks, based entirely on rugged silicon and some of its most stable and durable compounds. The approach offers a significant jump in efficiency without adding appreciably to large-volume manufacturing costs per unit, resulting in a corresponding decrease in installed system costs. The aim is to accelerate the development of this technology, to position it for industrial investment in its commercialization by the project’s conclusion (end August 2008).
Background

The University of New South Wales began photovoltaic research in 1974. After improving the $V_{oc}$ of “first-generation” wafer-based cells, it demonstrated the first of a series of “world records” for silicon cell efficiency in 1983. Apart from a six-month period at the end of 1988 (when Dick Swanson’s Stanford group produced a great result), it has held this record without interruption, improving cell performance by over 50% over this period. Many of these improvements are now in use commercially for space cells, and also terrestrially through the “buried contact solar cell”, developed at UNSW in 1984.

With sales of over US $300 million to date, certain to exceed US $1 billion by 2010, this has been one of the most successful commercializations of new solar cell technology over this period.

Spurred by the belief that silicon wafers were both too expensive and material-intensive to allow photovoltaics to reach the costs required to become competitive as a major energy source, the group commenced work on thin-film cells in 1988. As a preliminary, members visited several groups working on the key thin-film contenders. Then, as now, these were amorphous silicon (a-Si), copper indium diselenide (CIS), and CdTe. We formed the view that, like wafers, none had the potential to deliver on the long-term potential of photovoltaics. This was due to unattractive cost/performance trade-off, lack of materials availability and toxicity, respectively (subsequent experience has shown, additionally, that none are as stable as conventional silicon cells and may require special encapsulation (at extra cost) to produce the same level of field reliability, e.g. most recently. [1,2,3,4]

Encouraged by the developments in silicon cell technology, to which it had helped contribute, the group set about developing a silicon-based thin-film technology from the ground up (particularly important were developments in light-trapping, increasing the cell optical thickness, and in surface passivation, more critical as thickness reduces). The first factory for manufacturing these Si thin-film cells is now under construction (CSG Solar in Germany), with prototype product proving even more rugged in accelerated tests than conventional modules. [5]

With the impending success of this initiative, the group attempted to identify the features of the next generation of technology that it dubbed the “third generation”. The ultimate cost potential of the above-mentioned “second generation” Si thin-films is about half that of c-Si, low enough for PV to compete on the retail electricity market without subsidies. To compete on the wholesale market requires an additional reduction in costs. Apart from low cost, we identified a fundamental set of requirements for this third generation, specifically that it use abundant, non-toxic, stable and durable materials. This eliminates many technologies that are presently highly regarded.

The durability criterion also suggested that, as for second-generation modules, encapsulation would place fundamental limits on material costs (particularly glass and/or durable polymers). Hence, ever-improving efficiency (to improve the power from a given...
investment in material costs) was the long-term key to lowest-possible overall costs. After a detailed study of “third generation” concepts with prospects for boosting efficiency [6], the group identified a short-list that it felt had potential in the relatively short term.

Tandem or stacked cells of different bandgaps were at the top of this list as the most developed of the “third generation” options, since already used in spacecraft and in some amorphous (a-Si) thin-film modules. However, the former cells involve prohibitively expensive III-V technology while the latter modules, in the field, were likely to produce stable efficiencies of only 10% or so at best, not sufficiently high to leverage basic material costs.

Results

Administration


As described in the proposal, the work is divided between four strands: Processing; Characterisation; Modeling and Fabrication.

For the first year of the project the Characterisation and Modeling strands have been merged into one and, as the Fabrication strand involves construction of a tandem device, activity in this area will not begin until the second year.

Each of the two strands: Processing and Characterisation/Modeling are headed by a Research Fellow as strand leader. These two act under the overall control of the Principal Investigators.

The current stage of the research is on processing, characterisation and modeling of Si quantum dot nanostructures in dielectric matrices made by either sputtering or plasma enhanced chemical vapour deposition (PECVD).

Processing Strand

Tandem cells are stacks of individual cells with different energy thresholds each absorbing a different band of the solar spectrum, usually connected together in series. We aim to engineer a new silicon-based material to form a top cell above a silicon cell. This material is ‘engineered’ using a quantum dot nanostructure of silicon in a silicon based dielectric matrix. The confined energy levels in the quantum dots will increase the lowest absorption edge of the material compared to bulk silicon. If the quantum dot density is high enough the wavefunctions of the quantum dots will overlap to create true superlattice minibands and increase the effective band gap of the material.
The main challenge for a nanostructure engineered material for a tandem cell is to achieve sufficient carrier mobility and hence a reasonable conductivity. For a nanostructure, this would normally require formation of a true superlattice with overlap of the wavefunction for adjacent quantum wells or quantum dots; which in turn requires either close spacing between QWs or QDs or low barrier height. Another requirement for a tandem cell element is the presence of some form of junction for carrier separation. This can either be a grown or diffused p-n junction or a p-i-n junction formed in the superlattice as the i-region.

As reported elsewhere [7,8] such Si quantum dots have been fabricated by co-sputtering deposition of silicon rich layers interspersed with stoichiometric SiO$_2$ layers (an application of the method of Zacharias et al. [9] to photovoltaics). On annealing at 1100°C, silicon precipitates from the super-saturated solid solution to form nanocrystals. For layers of thickness less than about 4nm, our work suggests that the precipitation enters a regime of 2D diffusion in which the dot size is accurately controlled by the layer thickness.

The increased strength of optical processes in confined structures due to localisation of electrons and holes is highly advantageous for solar cell structures, as it means that only very thin layers of these dots are required for strong absorption. With an appropriate light-trapping scheme, thin films of unconfined Si of 1,000nm thickness give high solar absorption. Quantum dot devices of only 100 nm thickness seem feasible given the increased optical strength of the confined processes.

*Alternative matrices for Si quantum dots:*

Transport properties are expected to depend on the matrix in which the silicon quantum dots are embedded. As shown in Figure 1, different matrixes produce different transport barriers between the Si dot and the matrix, with tunnelling probability heavily dependent on the height of this barrier. Si$_3$N$_4$ and SiC give lower barriers than SiO$_2$ allowing larger dot spacing for a given tunnelling current.

![Figure 1: Bulk band alignments between crystalline silicon and its carbide, nitride and oxide.](image-url)
The barrier to tunnelling between quantum dots is reduced for a lower barrier height material, because tunnelling probability for a square potential well is given by, (e.g. [10] p244):

\[
T_c = 16 \exp \left( -d \frac{8 m^* \Delta E}{h^2} \right)
\]

where \( m^* \) is the bulk effective mass in the respective band of the matrix, \( d \) is the spacing between dots and \( \Delta E \) is the energy difference between this bulk band and the band formed by quantum dot interaction (\( \Delta E = \Delta E_c - E_n \)). Hence the important parameter in determining the degree of interaction between quantum dots is \( m^* \Delta E d^2 \). As barrier height decreases the barrier thickness for a given probability increases, thus requiring lower dot density for a given conductivity or higher conductivity for a given dot density. (In addition as dot size decreases \( \Delta E \) also decreases, thus increasing \( T_c \) and enhancing the effect further for smaller quantum dots.) [11]

Hence, transport between dots can be significantly increased as the barrier height decreases with alternative matrices. The spacing of dots would have to be closest in the oxide, nitride and carbide, in that order. Similar deposition and quantum dot precipitation approaches should work for all.

**Si quantum dots in a nitride matrix**

For the above reason we have explored application of similar techniques to those described above for SiO\(_2\), to the growth of Si nanocrystals in silicon nitride by both sputtering and PECVD. [12] For sputtering, growth parameters are very similar to the oxide but with growth from a Si and Si\(_3\)N\(_4\) target rather than from an oxide one. Results from HRTEM show crystalline nanocrystals in the nitride matrix.

In addition two separate PECVD machines have been used for the growth of Si nanocrystals in nitride, with a regime similar to that used in oxide, of growing alternate Si rich and stoichiometric nitride layers. Annealing is carried out again at 1100°C but with a pre-anneal at 500°C to drive off hydrogen incorporated from the PECVD process. Again HRTEM images showing even clearer nanocrystals have been obtained. [6] The two machines are a non-automated single plasma cluster tool and an automated dual mode RF/microwave plasma Roth and Rau machine. This demonstrates the transferability of the original approach both to other material systems and to other thin film processes.

Further optical and electrical characterisation is underway on these nitride materials. Other authors [13] have published data on Si QDs in Si\(_3\)N\(_4\) demonstrating crystallinity and increased PL energy but not using the close control of QD size that we have employed using the layering method. To the best of our knowledge this is the first time layered Si QDs in nitride / stoichiometric Si\(_3\)N\(_4\) samples have been prepared using either type of PECVD growth. The automated system also allows the possibility of growing large numbers of multilayers, which is important for several characterisation techniques. The approach is also being investigated for large area uniformity.


**Characterisation/Modelling strand**

In previous work several techniques have been implemented to improve characterisation of Si nanostructures. Complementary information from a range of techniques is necessary because the very small sizes of the nanostructures involved push the resolution of the techniques to the limit. Also complementary information on physical structure, optical and electronic properties is required in order to optimise processing.

**Physical characterisation**

The most routinely used of these techniques is High Resolution TEM (HRTEM) using a 300keV electrons and medium resolution (MRTEM) using 120-200keV electrons. MRTEM is useful for investigating the multilayer structure with indications of SiQD positions. With HRTEM, imaging of the lattice planes in individual Si QDs is possible. Examples of both are shown in Figure 2.

![Figure 2: a) MRTEM image at 120kV showing the multilayer Si nanostructure in an amorphous Si$_3$N$_4$ matrix grown by sputtering; b) HRTEM image at 300kV of Si quantum dots in nitride - showing individual lattice planes.](image)

HRTEM images showing Si lattice planes in Si QDs in both SiO$_2$ and Si$_3$N$_4$ matrixes suggest similar QD formation mechanisms in both dielectrics. Nonetheless TEM sample preparation is time consuming and not conducive to the fast feedback required for processing optimization. Hence new techniques for fast TEM sample preparation are being investigated. These include dual beam Focused Ion Beam (FIB) preparation, a double cleaving technique along specific crystallographic directions on the substrate and multilayer structure growth directly onto thin electron transparent silicon nitride films supported on a TEM grid.

Secondary Ion Mass Spectrometry (SIMS) is also used quite frequently through a collaboration with the Australian Nuclear Science and Technology Organisation, Sydney. SIMS gives compositional information with depth. Figure 3a is a SIMS plot of a Si nanostructure in oxide with detail of the Si and O traces on the right. It clearly shows the
alternating concentrations of Si and O in the multilayer structure. Figure 3b shows SIMS evidence for a similar multilayer structure for a nitride matrix.

Figure 3: SIMS profile of (a) SiQDs/SiO\textsubscript{2} multilayer structure on quartz substrate and (b) SiQDs/Si\textsubscript{3}N\textsubscript{4} multilayer structure.

Crystallographic information is obtained using Grazing Incidence X-Ray Diffraction (GIXRD). Two approaches have been used: analysis using X-ray tube diffractometers in the School of Materials Science at UNSW and analysis using synchrotron XRD at the Australian Nuclear Beamline Facility, Tsukuba, Japan.

An important aspect of the analysis is comparison of X-ray tube with synchrotron XRD data and comparison of both with information from TEM. Figure 4 shows two-theta plots for a Si QD in nitride sample. The sample has 20 bilayers of 10nm Si rich nitride layers. It shows that:
• The average Si nanocrystal size is 4.3nm – thus for this sample the SRO layer thickness was too thick to control the nanocrystal size.
• The lattice constant given by the \{111\} peak does not vary from the bulk silicon value by more than 0.1%.
• Deviation of intensities from random orientation are less than 10%.
The presence of crystalline Si is clear from these plots. In terms of quantitative analysis, the viability of both techniques for extracting average size, strain and lattice parameters of the nanocrystals is being examined.

Figure 4: Two Theta Plots of a Si QDs in nitride sample, using:
(a) synchrotron radiation and (b) a conventional x-ray tube source.

The peak positions and shapes are very similar between a) and b) in Figure 4 (except for the peak at 50° in b, which is a disallowed substrate peak), indicating that information that can be extracted from X-ray tube measurements is similar to synchrotron, at least at present. This is particularly true for the first peak at \{111\}. Information on average nanocrystal size is contained in the integral breadth or FWHM of the peaks. The less rapidly decreasing intensity with 2\theta for synchrotron is because synchrotron X-rays are polarised and the usefulness of this for detailed analysis of high index planes is being investigated.

Optical Characterisation – Photoluminescence (PL)
Photoluminescence (PL) is a key technique in assessing the energy levels within quantum dot structures. The highest PL intensities will be from the lowest radiative recombination states within the illuminated area close to the surface. Thus it is a tool which can assess whether quantum confined energy levels, greater than the band gap energy, are present. The fact that it can be applied to samples without contacts and with minimal preparation lends it to a quick turnaround feedback technique for processing. However, additional information with more careful analysis and at reduced temperatures...
can also yield specific detailed information on the stability of energy levels with
temperature and their relative luminescence intensities.

Figure 5 is a comparison of PL from Si QDs in a SiO₂ matrix for various layer
thicknesses and hence QD size with Si QDs in a Si₃N₄ matrix for a fixed layer thickness
of 4nm but with varying numbers of layers. PL measurements were carried out at room
temperature (300 K) using excitation by a laser operating at 405nm and 50mW with
detection by a thermoelectrically cooled Si CCD detector.

These results are discussed further elsewhere [12] and are tentative evidence for
quantum confined energy levels in Si QDs in nitride at a higher energy than in equivalent
layer thicknesses in oxide. However these are as yet early data. PL on various layer
thicknesses in nitride has not yet been obtained. These would show whether the 1.8eV
peak increases or not with decreasing layer thickness. In addition the intensity of the
nitride peaks is not high, probably indicating a low radiative transition probability.
Nonetheless the fact that intensity increases with the number of SiQD layers is
encouraging. Further data are being generated.

![Figure 5: Comparison of the PL spectra of Si QDs in nitride and oxide
(300K). Peaks on the left-hand side are for the nitride matrices. The higher peaks on the right-hand side are for the oxide matrices.](image)

Raman spectroscopy

Raman has been carried out on a range of SiQD in SiO₂ samples for various
percentage Si coverages. This percentage coverage is determined by the ratio of Si to
SiO₂ in the co-sputtering target. The results are shown in Figure 6.
Figure 6: Raman spectroscopy of annealed Si/SiO₂ multilayer samples for a range of values of percentage Si coverage (with the spectra of a Si reference sample and an unannealed sample for comparison).

The data in Figure 6 show that an increase in Si coverage results in an increased sharpness and intensity of the peak at 520 cm⁻¹. This is likely to be due to an increase in the proportion of crystalline Si which has a Raman shift at 520 cm⁻¹. The significance of the asymmetric broadening of this peak and other possible peaks is being analysed but may well contain further information on the nanostructure.

Electrical characterisation

Electrical characterisation has so far concentrated on lateral conductivity measurements. Although vertical measurements are the more relevant for structures of interest, lateral measurements are easier to model because they only involve transport within layers containing Si nanocrystals whereas vertical measurements include both intra-layer and inter-layer transport across the intervening oxide layers.

Contacting for lateral conductivity measurement has been achieved by using a technique of using Al contacts to ‘punch’ through the surface oxide, by annealing evaporated Al at 500°C for 15 hr. This induces non-uniform spiking through the upper layers of oxide and provides a very large surface area contact to the QD layers, as shown in Figure 7. This in turn results in a voltage drop across the contact about a factor of 10 lower than the voltage drop across the active region of the Si QDs, thus resulting in a small relative contact resistance, R_c.
**Figure 7:** Schematic of sample structure for lateral conduction measurements.

Figure 8 shows current conductivities for a range of Si concentrations in the Si rich oxide layers. It shows that conductivity generally increases as Si concentration increases, probably because of an increase in carrier transport as the average distance between neighbouring Si QDs decreases. Such transport would either be via a direct tunnelling mechanism through the oxide or by hopping via defects in the oxide. This has been investigated further by measuring conductivity against temperature. The slopes of the data in Figure 9 shows lower conductivities than that from [14] particularly at higher temps, although at 300K there is reasonable agreement. Work using this technique is reported elsewhere. [15]

**Figure 8:** Conductivity of SiQD in SiO$_2$ samples for various %Si contents. (Al contact spacing is 300 µm. All samples had 20 bilayers of nominally 5nm SRO and 10nm SiO$_2$ layers.)

**Figure 9:** Plot of conductivity vs. temperature for Si QD sample in SiO$_2$ for a 55% Si coverage as compared to data from [14].

**Modelling**

Modelling is important for the interpretation of characterisation data and for designing new structures and experiments. In 2005 modelling techniques have been developed further, with additional improvements expected to continue.

Effective mass approximation (EMA) approaches are being used to model expected confined energy levels in experimental structures. The EMA approach is being extended to include effects of non-uniform QD size as well as inter-QD distance. This will result in
a more realistic modeling of the transport properties as a complement to IV characterizations. The statistics of the QD size and inter-QD distance will be obtained directly from HR-TEM, and indirectly by X ray diffraction (XRD) and photo luminescence (PL), e.g. as shown in the XRD data in Figures 10 & 11.

**Figure 10:** XRD for a sample with 62 bi-layers (each 4.5 nm SiO$_{1.45}$/3 nm SiO$_2$) and a reference substrate.

**Figure 11:** Differential XRD spectrum of Fig. 10, showing all diffraction peaks for the 62 bi-layer sample containing Si QDs. FWHM gives $d_{QD} = (44.8 \pm 6.1)$ Å.

On reduction of the Si QD size, the effective band gap increases and the effective mass approximation becomes increasingly inaccurate. First calculations of the energy levels using ab-initio calculations based on the density functional Hartree-Fock theory (DF-HF-T) were carried out by using the DF-HF software Gaussian03 [16]. These will be compared to experimental data and EMA solutions. The electronic structure of hydrogen (H) terminated non-periodic Si QDs with optimized spatial structure have been calculated. Their highest molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies correspond to the valence and conduction band edges in the EMA picture, as shown in Figures 12 & 13.

**Figure 12:** HOMO and LUMO level of single H-terminated Si QDs as a function of their diameter $d_{QD}$.

**Figure 13:** Effective band gap of single H-terminated Si QDs as a function of their diameter $d_{QD}$.

Ab-initio calculations are expected to be a powerful tool in modelling a wide range of potential structures.
HRTEM remains the most powerful technique to examine these materials at sub-nanometre resolution. It is important to remember, however, that the image formation system of the TEM is not perfect. The information contained in the diffraction pattern of HRTEM extends much further in reciprocal space than is accessible by the microscope. The contrast transfer function contains zeros and inversions meaning that some spatial frequencies present in the sample are not observed in the images and other spatial frequencies are imaged with reversed contrast. Essentially nanoscale imaging is beyond the resolution limit of the TEM microscope but is not beyond the information limit. Hence careful modeling and simulation of the TEM artifacts can enhance a naïve interpretation of TEM diffraction data.

To examine the image simulation process, a large number of images of particles of various sizes, shapes and orientations have been performed and a library of images is being generated. This will form the basis of an image-matching system which will be able to identify particular crystal structures found in experimentally acquired images.

**Progress**

Widespread implementation of renewable energy would reduce the reliance on fossil fuels and substantially reduce the emission of CO₂. Photovoltaics is the most versatile and modular renewable energy technology and the most applicable for small scale retrofit or new build implementation at the local distributed generation level. The technology involves close to zero greenhouse gas emission at the point of use and low embedded energy and hence greenhouse gas emissions. Barriers to implementation include the presently uncompetitive initial investment cost of photovoltaic modules as compared to conventional electricity delivery via the grid for each peak Watt of installed capacity.

Routes to decrease this ‘cost per Watt’ are either to reduce the cost of the technology or to increase its efficiency. The first of these is addressed by the use of thin film technology for low cost deposition at relatively low temperatures and with low material usage. The second is addressed by using multiple threshold devices to push efficiencies beyond the Schockley-Queisser limit for single band-gap photovoltaic cells.

Since its start in September 2005, the current project has begun to make progress towards the objective of a low cost but also high efficiency tandem photovoltaic cell based on silicon and its compounds. Specifically this progress includes:
- The appointment of new staff members;
- Further development of the transfer of SiQD growth from oxide to nitride matrices;
- Extension of Thin Film growth techniques from sputtering and PECVD to large area PECVD;
- Development of characterisation to include XRD of Si nanostructures and further development of SIMS and TEM techniques and modeling;
- Further development of optical characterisation techniques, e.g. Raman and PL, and of electrical characterisation;
• Development of modelling capability including ab-initio calculations of Si QD confined energy levels with complex atomic structures and highlighting the limitations of the effective mass approximation [17].

**Future Plans**

Commercially available deposition techniques will continue to be used to fabricate Si quantum dots in matrices of nitride and carbide, for example, sputtering, chemical vapour deposition (CVD) and e-beam evaporation. For formation of self organised Si QDs in SiC, Si$_{1-y}$C$_y$ alloys with 0 < y < 0.5 are thermodynamically metastable and may therefore be synthesized to quantum dots in a growth process involving post growth high temperature annealing. The bandgap of the silicon carbide is expected to depend on the carbon content in the film. [18]

Also we will investigate a modified quantum dot formation process by means of high concentration of atomic hydrogen in the plasma. Nano-crystalline silicon can be deposited from silane plasma that has been heavily diluted with hydrogen. It is possible that atomic hydrogen will permeate the film of amorphous Si-Si bonds, lowering the energy barriers to the rearrangement of the silicon network into a more stable and ordered nanocrystalline lattice. Silicon quantum dots in silicon nitride grown by NH$_3$ and Si$_3$H$_4$ potentially eliminate the post high temperature annealing process, which is presently required, giving more flexibility in device design. [19]

Another approach is for hydrogen reactive sputtering of carbon and silicon to form SiC nanocrystals, again eliminating the high temperature annealing process. [20] Fabrication of silicon quantum dots in a silicon carbide matrix and observation of quantum confinement will be the aim of this part of the project. In addition doping from n-type or p-type precursors will be investigated for future photovoltaic device fabrication.

The QD p-i-n cells are essential for the final device. Given the strong absorption by QDs, these cells can be thin around 100nm to 1µm allowing a cell structure design with a depleted i-region. This relaxes requirements upon carrier mobility since collection is field-assisted. Graded bandgaps by grading QD size may also provide complementary design features. Design parameters for the fabrication of the tandem photovoltaic cell will also be investigated during the next period.

**Photoluminescence**

In the silicon oxide matrix, trapping of an electron by the silicon-oxygen double bond is thought to produce localised levels in the bandgap of the quantum dots. [21] Photoluminescence will be used to investigate these silicon-oxygen double bond states in silicon quantum dots in the oxide matrix fabricated by RF magnetron sputtering.

**Electrolytic CV**

We are currently pursuing the re-commissioning of an electrolytic CV system. This would enable us to investigate the charge state of QD arrays and the electrical quality of the QD/dielectric interface as well as of the dielectric itself. Using an electrolyte electrode would spare the need to use metal evaporation for top electrodes of the samples. This is not only useful for avoiding any change of the ultrathin QD layers by
unintentional incorporation of metal atoms, but also provides the flexibility to measure in any location of the sample. The latter can be exploited for obtaining a full statistical data set, e.g., by sample mapping.

**Hall effect**

We are also currently establishing a Hall effect measurement system. This will be used for high precision Hall effect, mobility, and carrier concentration measurements in addition to being useful for determining tunneling characteristics for electrons with a k-vector exclusively perpendicular to a tunneling barrier in single QD arrays and QD superlattices.

*Ab-initio DF-HF calculations of Si nanostructures:*

A Beowulf type Linux computer cluster consisting of 40 AMD Opteron 64 bit 2.2 GHz CPUs and a cumulative 44 GB RAM is currently being established. Its projected computation power of 100 G-FLOPS provides the hardware for detailed ab-initio DF-HF computations of nanostructures.

With the purchase of the ab-initio DF-HF software mentioned above [16] we are able to compute the structural, energetic, optical, and phononic properties of nanostructures involving QDs consisting of Si and other solids with an effective band gap in the range of interest. There are two major objectives:

Ab-initio DF-HF computations deliver precise results of the properties mentioned above for a wide range of chemical compounds, thereby presenting a means of predicting the properties of certain material configurations (like Si QDs in an imbalanced SiC dielectric matrix) or potentially attractive solid compounds like Ge QDs in a SiC dielectric matrix.

Computing structures for which experimental results have been obtained serves as a complementary method of model building. Certain PL peaks which do not seem to depend on the QD size may serve as an example. In this case, the ab-initio DF-HF computations can clarify whether these size-independent PL signals are due to radiative point defects being located within the dielectric matrix, at the interface of the QD to the dielectric or—rather unlikely—within the QD. Inter-QD coupling and phononic engineering of materials are other attractive issues.

**Publications**

References

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