Quantum Generative Modelling of High-Performance Quantum Dots for Solar Harvesting

A strategy to discover new quantum dots with optimal properties for sustainable solar harvesting

Background:

In the face of rising energy demand and the depletion of fossil fuels, researchers are turning to clean, renewable alternatives like solar power. Photovoltaic (PV) technology, which converts sunlight into electricity using semiconductor materials, offers a promising solution. When light strikes these materials, it frees electrons and generates electrical current. However, conventional silicon-based PV cells remain costly and limited in efficiency, prompting innovation toward more advanced, affordable technologies.

One breakthrough is Quantum Dot-Sensitized Solar Cells (QDSSCs), which use nanoscale particles called quantum dots to absorb a broader spectrum of sunlight. Theoretically capable of reaching 44% efficiency, far surpassing traditional solar cells, QDSSCs work by separating charge generation and collection processes, minimizing energy loss. Recent experiments have achieved 17% efficiency with improved quantum dot coatings, showing that this technology is moving from concept to reality. Though challenges like charge recombination losses and environmental impacts remain, QDSSCs hold strong potential for delivering cleaner, more efficient, and accessible energy in the near future

(Z. Yang, C.-Y. Chen, P. Roy and H.-T. Chang, “Quantum dot-sensitized solar cells incorporating nanomaterials,” *Chemical Communications*, no. 34, 2011.)

Purpose: Develop quantum technology targeting the Sustainable Development Goals

The goal of our project is to develop a strategy for generating new quantum dots with a given set of properties (described below), and the motivation behind this goal is the

UN Sustainable Development Goals (the SDGs). Research on quantum dots in solar harvesting is ongoing, and some of the big challenges are avoiding toxic materials and increasing efficiency. These challenges directly relate to SDG 7: Affordable and Clean Energy and SDG 13: Climate action. Solar power is a vast, but poorly exploited renewable energy source, and improving the efficiency and viability of solar harvesting technology could be an important step towards affordable and clean energy across the globe. Clean alternatives are necessary to drive the transition away from energy production methods that are harmful for the climate, thus our project is also a climate action initiative. In addition, reducing the use of toxic elements is crucial for the technology to be environmentally reasonable/responsible as well as scalable considering regulations on emission of toxic elements in nature. This can be related to SDG 12: Responsible Consumption and Production, focusing on e.g. non-harmful production lines. Another relevant SDG is SDG 9: Industry, Innovation and Infrastructure, as the photovoltaic field has the potential to grow into an even more important industry in the future depending on innovative solutions today. Finally, it is also desirable that the quantum dots are produced with available, non-expensive materials so that the technology can be affordable.

Enhancing Solar Cell Efficiency through Quantum Dots and Emerging Photovoltaic Technologies

Supercharging Solar With Quantum Dots - WSJ

Goal properties: Desired properties of a high performing quantum dots

- Band-gap: 1.2–1.8 eV or 1 μm (near-infrared) to 700 nm (red). This band-gap can complement existing band-gap of traditional tandem solar cells (1.1 eV) and maximize current while keeping the open-circuit voltage high. (Halide homogenization for low energy loss in 2-eV-bandgap perovskites and increased efficiency in all-perovskite triple-junction solar cells | Nature Energy)
- Absorption coefficient: > 10^5 cm^{-1} at 600 nm, in order for 90% photon absorption to occur and comparable with the typical size of photovoltaic absorber layer, which is around 200 nm to 1 μm. (https://doi.org/10.1016/j.solener.2019.12.014)

- High photoluminescence quantum yield (PLQY, >50%) to reduce nonradiative recombination and thus can potentially increase the efficiency of the solar cell. (High Photoluminescence Quantum Yield in Band Gap Tunable Bromide Containing Mixed Halide Perovskites | Nano Letters)
- Non-toxic materials (no Pb, Cd), e.g., InP, ZnSe, $CuInS_2$, or Pb-free perovskites are preferred to align with SDG 12.

Method: Hybrid quantum classical QCBM

Since quantum dots are quantum mechanical systems, a quantum machine learning method might be well suited to capture underlying quantum structure and regenerate it in new quantum dot candidates. It is expected that quantum generative models are more efficient than classical counterparts in situations where the available data is limited, but highly (quantum) structured. This is the case for quantum dots. Several studies have shown promising results for QCBMs compared to classical methods.

Implementing Quantum Generative Adversarial Network (qGAN) and QCBM in Finance

https://arxiv.org/pdf/2311.05050

https://pubs.acs.org/doi/pdf/10.1021/acs.jcim.3c00562?ref=article_openPDF

Figure (1) shows a schematic of our hybrid quantum classical model. An autoencoder reduces the data describing the quantum dot structure to a three-dimentional latent space. A generative quantum circuit Born machine takes this as input and outputs new values for the same three features which are subsequently decoded by an autodecoder. The idea is that based on the decoded output, a new quantum dot candidate can be reconstructed. The most promising candidates (based on the model's estimate of the candidate's properties and after rejecting those containing toxic constituents) will be FDT simulated to determine to what degree it meets our property criteria.

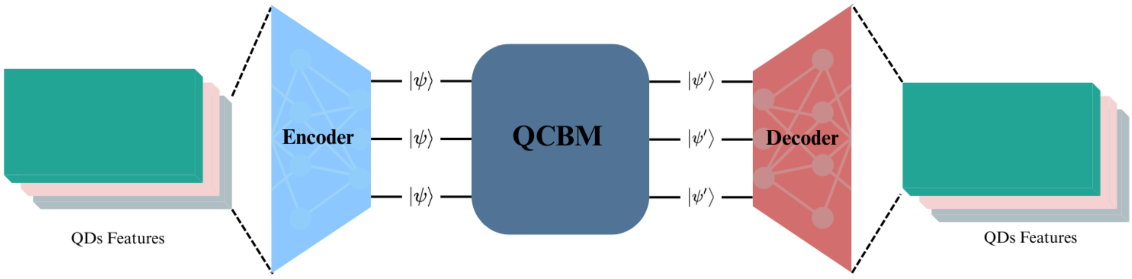

Figure 1: Schematic of the hybrid classical quantum model. The encoder-decoder pair is classical, whereas the QCBM is a parametrised quantum algorithm.

At the early stages of this project, the available data is to a large degree based on quantum dots that do not meet our criteria, so we expect that many of the generated candidates will be rejected. The few good data points existing will be weighted by our model in the following way: The quantum circuit Born machine is a quantum algorithm that can be trained to reproduce a probability distribution. Therefore, the input data has to be expressed as a probability distribution over the available data points, expressed as bitstrings. If we want the model to weigh the different input data points differently, we can assign them different values in the input probability distribution. Otherwise, we would use a uniform distribution. Through tuning the trainable parameters of the quantum circuit, the model learns to output bitstrings (represented as quantum states) that have similar underlying structure as those with non-zero probabilities in the input distribution. In this way, the model generates data points that are similar to the input data points, which is what we want. Repeating this a large number of times, the model creates a discrete probability distribution over the output bitstrings, and the output bitstrings that were not among the input bitstrings are new quantum dot candidates.

Dataset: Collecting what we can find

The goal is to train the model on structural data of known quantum dots used in solar harvesting. Obtaining complete structure data of known quantum dots is difficult since these are often not publicly available due to the commercial aspect of the field. As a result of this, we have instead tried to collect the information listed below about each quantum dot from a selection of sources including The Materials Project and this overview:Quantum Dots - CD Bioparticles.

- Composition of the core
- Type of ligand
- Composition of shell (if applicable)
- Structure constants for the core
- Band gap
- Quantum yield
- Volume and density of core
- Diameter of nanoparticle
- Emission maximum

Due to our chosen autoencoder/decoder structure, the format of the output data will be the same as the format of the input data. Since we need the output of our model to contain enough information to reconstruct a quantum dot structure for DFT simulation, we also need this in our input. It is also necessary that the input data contains enough information about the quantum dot so that it is possible for the quantum machine learning model to extract useful information about their common underlying structure. So far, we have started to collect this data, but it needs to be verified, improved and extended. In order to develop and test a code example for the model, we have used a synthetic dataset containing the desired information for a fake set of quantum dots generated by chatGPT.

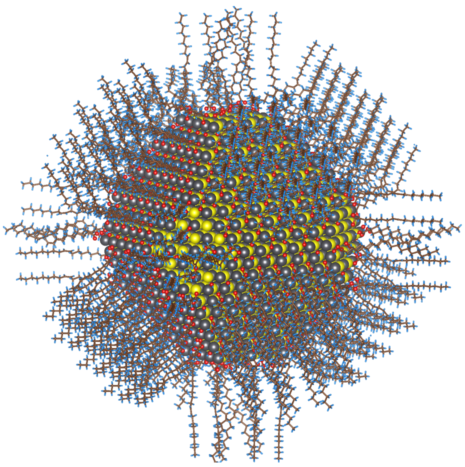

Figure 3: A visualisation of a quantum dot.

Three stages of quantum dot generation: a short and long term strategy

Stage 1: What can be done now?

Use available data on quantum dots to generate quantum dot candidates to be validated by DFT simulations. Due to limited available data, we use all available data of quantum dots used in solar harvesting to generate quantum dot candidates without (much) concern of the property constraints above. Among the generated candidates, we reject the ones containing toxic constituents. The good candidates are DFT simulated to evaluate if they meet the criteria for band gap, absorption and quantum yield. One research question that we have not had time to investigate is how we can determine if a candidate is good or bad without doing the full simulation. If we have input data for the constraint variables, we would also have an estimated output value for the feature. We could then use the (approximate) model estimated constraint properties (like band gap) to determine the "goodness" of a suggested candidate, meaning that the candidates with a good estimated band gap for example, would be DFT simulated first. This is a (probably non-efficient) process to start building up the data we need for more efficient candidate generation in later stages, and also, hopefully, to discover some valid candidates for high performing quantum dots. When a quantum dot candidate satisfying the constraints above has been suggested, simulated and thus validated, the first stage of our project will be considered completed. However, there are still important considerations to be taken into account before we have a candidate ready for testing concerning e.g. availability of the material, viability of its production and its cost since this is not evaluated by the model. That being said, in the first stage of the project, the goal is primarily to generate good candidates that can be used for more efficient candidate generation in the next stage, so even non-feasible candidates are considered good results.

What is needed:

Steps	Status	Challenge
A dataset describing the structure of known quantum-dots for solar harvesting	started collecting data from articles and materials project	this is a slow process and much data is not openly shared
A classical autoencoder to reduce the data size	we have a test version	need testing to verify how well the information is represented in the latent space/ balance with #qubits available
A quantum generative model that extracts underlying structural information about the quantum dot	have a test version	needs refinement
Reconstructing the nano particle from the decoder output		
Pre-sorting: toxic or not	easy to implement	
DFT to simulate band gap, absorption and	have done literature search to confirm	time consuming and difficult

quantum yield of candidate to validate or discard it	feasibility and availability of software for our purpose and it seems okay	

Stage 2: When the stage 1 procedure works and has given good results

After having accumulated a set of good quantum dot candidates through stage 1, this data can be used to make the generating process more efficient. If the training data consists of only (or at least more) good candidates, hopefully the post-processing rejects fewer candidates. The model will also be altered based on observations and discoveries during stage 1. In this part of the project, the goal is to generate enough good quantum dot candidates so that some of them are also feasible taking into account availability, production and cost.

What is needed:

- An accumulated dataset of good candidates
- An improved model

Stage 3: Imagining the future

In order to fully exploit the power of studying a quantum system with a quantum computer, one intuitively promising idea is to avoid the intermediate step of extracting a (non-complete) classical description of the innately quantum nano particle through measurement and then ("artificially") encode the classical information as a quantum state. To do this, we would need a direct quantum mechanical representation of the nano particle, meaning that a physical nano particle would have to interact coherently with some kind of quantum system that is able pick up (some of) its defining properties (without strictly copying it since this is forbidden by the no-cloning theorem). This quantum state would be the input of a similar generative quantum machine learning model as the one explained above, but without need for any encoding. Arguably, by the time this is technologically possible, the number of logical qubits available in quantum computers is also higher, so the autoencoding might also not be necessary. However, a number of technological challenges remain to be tackled before this would be a realistic possibility: e.g. avoiding decoherence effects, obtaining quantum memory to keep the input state across several training epochs and how to effectively encode the nano particle state as qubits (or qudits) to name a few. Without having spent time on exploring the challenges and possibilities of this idea in detail, we leave it here as speculative food for thought.