Optimization for Quantum Dot nanoparticles

ENGR 132 Design Project

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by

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Table of Contents

Design Process Step and Documents Page/Tab

|  |  |
| --- | --- |
| **EXECUTIVE SUMMARY** | 3-4 |
| **M1 SUMMARY** | 5 |
| **M2 SUMMARY** | 5 |
| **M3 SUMMARY** | 5-6 |
| **M4 SUMMARY** | 6 |
| **M5 SUMMARY** | 6-7 |
| **M6 SUMMARY** | 7 |
| **M7 SUMMARY** | 7 |
| **M8 SUMMARY** |  |
| **M9 SUMMARY** |  |

Executive Summary

(Completed during MS9; 1-2 pages)

We are partnering in this endeavor with nanoHUB. We are developing a simulation suite that helps our clients visualize certain aspects of the photovoltaic panel fabrication process, as it relates specifically to quantum dot nanoparticles. For the direct user (the PV fabrication team), our goal is to provide them with a way of easily testing different ‘recipes’ for mixtures of QD materials in order to achieve a given average band gap energy. The solution we have arrived at is a system equations an calculations that decide which of the materials entered by the user are the most effective for reaching the desired band gap energy. Based on those selections as well as the other data supplied by the user, we then build a ‘recipe’ to attain the goal band gap energy. We used this model and with some small adaptations to create a system of several GUIs that allow the user to navigate and interact with push buttons, edit text boxes, pull-down menus, check boxes and sliders. They will enter data as prompted and then the GUIs will calculate and plot the information enumerated in their descriptions. The main purpose of the suite is to use the model described above to allow the solar cell fabrication team to rapidly test the feasibility of a particular set of materials and attributes. We see this simulation suite as the first level of testing and prototyping in the creation of a new quantum dot solar cell compound. Our simulation consists of three computational GUIs and several support windows. The GUIs can be accessed individually from a main menu via push buttons. The lowest level of ‘magnification’ is a GUI that takes the data entered and computes the best ‘recipe’ based on the information entered in the data entry GUI (which can be accessed from any of the simulation windows as well as the main menu). This simulation also displays the optimization curve based on the weighting supplied by the user. This GUI allows the user to print out a physical copy of the graphs so that it can be more easily shared. The next deeper level is a GUI that looks fairly simple but is designed as a ‘catch’ for factors that weren’t included in our base simulation but could still be important to the user. This GUI has additional entry fields for any material attribute that the user wants to enter. It then applies those attributes to the materials that have already been entered and creates an optimized recipe and allows the user to display the original recipe, then the recipe optimized for each of the four auxiliary attributes. The auxiliary attributes can be plotted together in any combination desired. A weakness of the simulation is the way that it optimizes the attributes. It may not be viable for some additional attributes that the user would like to input. The final and most customizable layer of detail is a GUI that lets the user choose any of several combinations of factors that affect the materials and plots up to three of them together in the same window in a variety configurations. This lets the user see how a single factor or attribute is affected by the others. A potential weakness with this simulation is one of its greatest strengths, its high level of customizability. It could be difficult for the user to find the combination of factors that would be most useful to them. For all the GUIs we have supplied help windows that describe the use of the GUIs and what the user is expected to enter and select and how each of the simulations behave.

Our definition of success in this project is a fully functional suite of interactive visual simulations that allow our direct user to get an idea of how effective a given ‘recipe’ of quantum dot materials is at achieving a particular goal band gap energy. We believe that our suite is well suited to our intended audience of fabrications teams for solar cell manufacturing companies. Our aim when designing the interface for our simulation was to create a very bare bones presentation that would communicate the data as quickly and clearly as possible. We also tried to make our simulation as open ended as we could, allowing for factors that we may not have foreseen coming into play. The general design scheme was built around the idea of a microscope. Each of our GUIs is a higher magnification into the field. Each gives a different layer of detail, some more focused, some broader in scope and adaptability. We did this by creating a mathematical model that accomplished our general goal of minimizing a numeric attribute of a particular set of materials and returning the best ‘recipe’ to produce the desired output. From there we adapted and augmented the model so that it fit the needs of our individual simulations. They are built on the same premise, “the user wants to create the best ‘recipe’ possible from this set of materials,” but they approach it from different angles. As we tailored our solution to the target audience and their needs, we saw that some of our initial ideas were not as applicable as we thought. This led us to change some of our ideas, consolidate and unify some of the presentation. A weakness we see in our suite is its relative simplicity. While it does present the desired output, it is not able to provide great detail in its solutions. Another weakness that was unavoidable is the platform on which it was created. Matlab is an excellent numeric environment, but that strength does not spill into GUIs. Matlab GUIs, while functional, are not the most elegant or user friendly. This factors greatly into every aspect of our simulation. How our direct user interacts with our product, how our model interacts with the user through the environment of the GUI, how our visual representations of the data are achieved and possible most importantly how our user interacts with the GUI itself. We have added as much interactivity as we could and was appropriate to the specific applications of our models. It would make little sense to add a rotate feature to a two dimensional graph. In addition the ability of the user to alter the data is a bit clunky by very nature of GUIs in Matlab. We combated the bulkiness of the system by designing the flow of our GUIs in such a way that the individual simulations talked to each other, transferring the data between them so that the user would not have to enter the same data multiple times. As well as adding help windows and pop up error boxes to guide the user in correctly using he simulation.

Milestone 1 Summary

The outcome of Milestone one was a collection of information relating to the development and implementation of PV Quantum Dot technology. Briefly, the information contained in the document is organized as follows. The initial section is a reflection on the problem at hand, what is needed? By what are we constrained? For whom are we making this product? The second section is a list of potential stakeholders in PV technology, as well as a description of each and whether or not that particular party would be in direct contact with our proposed product. We were then asked to evaluate our list of stakeholders and narrow it down to one particular primary direct user for whom we would be specializing our simulation suite. Once we had picked one and given our reasons for doing so, we then researched and brainstormed about what we would need to know in order to create a simulation suite that would actually be useful to our chosen user. The end goal of this milestone was to narrow down the end result of the project, to force us to think about and research our direct user, so that when it comes time to actually produce the suite, we will have the information necessary to develop a set of simulations that have a direct correlation to the needs of the user.

The main feedback that we received was directed at our oversight as far as citations and proper formatting.

We addressed these concerns by properly formatting our citations and including correct in-text attributions.

Milestone 2 Summary

Milestone two was an assignment that was designed to elicit from our team a further distilled list of the concepts and ideas that had been generated in the previous Milestone. In short, Milestone two is organized according to the following description. The first section of Milestone two is devoted to a short recap of Milestone one, the feedback we had received from the peer team and how we planned to address it. The next portion is a table where we catalogued more than a score of concepts that we thought would be viable simulations, either freestanding or combined with one or more other concepts from the list. Within each idea, we also communicated the evidence we had found as to why this concept was useful. There were also associated boxes for the sources we had discovered in our research, the concept generation strategies we had implemented, as well as for the specific user criteria we deemed individual concept addressed. Following that segment was another table set aside for our full APA formatted citations (in alphabetical order), as well as a space for a few lines from each member describing their individual contributions to the Milestone.

We received very positive feedback on our work for Milestone two. The reviewer did not have any critiques concerning either our content or formatting. Pursuant to this favorable assessment we did not make any changes to M2 and attempted to apply our previous standards to the current Milestone.

Milestone 3 Summary

Milestone 3 was again a continuation of the previous two milestones. This milestone, however, differed from those before. This milestone the documentation of our path to condensing our set of twenty ideas down to a suite of four graphical user interfaces that are related in some way to each other and all correlate to the desired goal of developing a simulation suite that assists our direct users (the fabrication team for a solar cell manufacturing company) visualize data that pertains to their mission. We did this in several ways. We initially voted on each of the twenty concepts, each member had one vote, and when we finished voting for the ideas we eliminated the lowest ten ideas and then discussed each of them. We used the supplied pro/con tables to evaluate each of the ten ideas, citing our sources and using documented and cited rationale for how we weighted each of the pros and cons. We then assigned each of the ideas a weighting between 1 and 5. When each idea had been weighted and summed the scores were compared and four best results were selected as our final simulation ideas. Then, for each idea, we each selected one that we were going to be responsible for coding in the end graphical user interface GUIs. When we had determined who would be coding what, we each wrote a paragraph describing how each GUI related to the main purpose and to the other GUIs (each was written with input from the other team members). We each then wrote our contribution statement at the end of the document.

We received good feedback on M3 for the most part. However, there was concern with our rationale for the pro and con table, we had carefully devised a system of rationale that could be extended to each of the ten ideas, the apparent desire for the grading team was that there should be distinct rationale for each idea, this was not communicated and we felt it to be unnecessary given the information that was made available to us when we generated these rationale.

We evaluated the feedback, but as we are not re-iterating M3 there is not a place to communicate our changes other than in this document. We do not feel that the rationale was inappropriate or that the tactic we used by employing the same rationale for all weighting was against course policy. We do however, wish to communicate our desire to conform to the desires of the grading team. We feel that there would be a better chance of success if the grading rubric were supplied for all assignments before the due date, so that those completing the assignments know exactly what the graders are looking at, so the students can achieve the best result possible given their abilities and their desire to complete the requirements in the most satisfactory manner possible.

Milestone 4 Summary

After our presentation of M4 we received minimal feedback, most of it related to aesthetic/organizational elements. We were told that the basic premises of the GUI simulations were good, but perhaps a little cloudy on what their purpose was. We feel the presentation was a success, in preparing for it and discussing it afterwards we discovered a few things that we wanted to do differently.

From the feedback we were given, we decided to include a couple extra buttons in the GUIs that would allow the entry of new data, or the use of the original data set that we are now allowing to be entered via the main GUI window.

We have taken these things into account and have edited our slides/pseudo GUIs accordingly. We feel that our simulation is robust and will be useful to our direct user.

Milestone 5 Summary

Milestone 5 was simply a resubmission of M4.

The feedback we received was mostly positive but there were a couple of concerns with our citation methods the requirements for which were unclear. There was also mention of a couple of our GUIs being too similar, that was an error in our description, the surfaces present information in a similar format, but have different outputs, while the layouts look the same the information is different.

We have looked over these concerns and will attempt to rectify them to the best of our abilities.

Milestone 6 Summary

Milestone 6 was the first submission of our simulation suite. It was our first iteration of the suite and was geared more to give an idea of what our GUIs would look like than for functionality. All the buttons worked and the control of the program moved between them as the navigation buttons were pushed.

We received very positive feedback on our work for M6, the only thing the grader mentioned was a small lack of uniformity between the navigation buttons, and different naming conventions had been used and not edited. There was also mention of the need for help windows. The other comments were more towards cosmetic issues, most of them stemming from a misconception that we were intending our suite for a younger less professional audience.

We have addressed the major feedback and cleared up the misunderstanding about our design aesthetic. We standardized our displayed buttons names and made them as uniform in window placement as we could, given the differences between our respective GUIs. We also added help windows with information about the use of our GUIs where necessary.

Milestone 7 Summary

Milestone 7 was a success. The main purpose of M7 was to demonstrate some functionality in our GUIs as well as fully functional navigation buttons. We received good feedback on our efforts. The only concern that was addressed by the reviewer was some inconsistency in our naming conventions. Some of our supplementary files were not named according to the proscribed standards. The one other note that was made was our lack of in-text citations.

As for our deviation from naming standards we have altered the filenames to conform to the standard. We are unable, however, to abide by the request for in text citations as all of our citations are related to our layouts themselves and fall under the category of ‘prior art.’ By their very nature it is impossible to include in-text citations in pictures or GUI layouts. We made an attempt to note this fact before we submitted the milestone but the grader apparently didn’t look at our source code for the explanation we left.