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RE: Optimizing a Mixture of Quantum Dots for a PV Customer

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**Part 1, Introduction**

According to the information provided to our team, we have come to the conclusion that the direct user of our deliverable will be the manufacturing department employees. The direct user primarily needs the deliverable. The deliverable is the model or algorithm to determine the solution of the problem that has been presented. The function of the deliverable is to either run simulations of or perform calculations for a variety of applications within a certain scope, providing actionable data for those researching and evaluating possible solutions or products. Some of the criteria by which the success of the model could be judged are: its ease of use, the efficiency of the deliverable, the cost effectiveness of the deliverable and the versatility of the product. A few of the more important constraints on the system could be: the amount of time it takes for one iteration of the process, the cost of the deliverable, the amount of data that are needed for input or result from the process as well as the ability of the deliverable to address the possibly widely varying needs of the program for which it is designed.

The model requires several key data points such as the dielectric constant of the materials available, the radius of the Qdot of the materials available, the bulk band gap energy of the materials available, the desired Qdot energy of the product material. Based on these and given for which characteristic(s) to optimize, it will create an optimal combination of the available materials to be used for manufacture.

We believe that our model will be useful under a variety of circumstances, but primarily with the intent to minimize the cost/toxicity level of a given material. The model functions best when only one variable is allowed to change per iteration.

**Part 2, Procedure (mathematical model)**

Our model assigns value to each of the materials. Given the band gap energy, , is a weighted average of the component materials and the average cost per gram or toxicity per gram, , is also a weighted average, we can define a quantity called value that represents the “cost efficiency” of the material, .

It then selects the most valuable material with a band gap energy greater than the goal for the product and the most valuable material with a band gap energy less than the goal. It then augments the minimum with usage requirements (in this specific case 2%) with these two materials to achieve goal band gap energy. It uses the following system of equations to determine this:

Where is goal band gap energy; and are the band gap energies of the most valuable material over and under the goal, and are the mass fraction of these two materials necessary(over the minimum); is the band gap energy of the th material; is the minimum usage requirement by mass fraction; and is the number of materials.

The first equation is merely a rewriting of the formula for the band gap energy of a combination of materials with known band gap energies. The second merely states that all the mass fractions should add up to a whole.

The justification for this method can be found in the supporting materials.

**Part 3, Results**

Using our model we have determined the cost optimized methods to create 100g of product are as follows:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Band Gap Energy | Material 1 | Material 2 | Material 3 | Material 4 | Material 5 | Cost |
| 1.33eV | 2g | 2g | 61.14g | 2g | 32.86g | $2754.28 |
| 1.65eV | 2g | 2g | 12.02g | 81.98g | 2g | $3799.68 |

Using our model we have determined the toxicity optimized methods to create 100g of product are as follows:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Band Gap Energy | Material 1 | Material 2 | Material 3 | Material 4 | Material 5 | Toxicity (impact) |
| 1.33eV | 2g | 2g | 2g | 29.19g | 64.81g | 176.81 |
| 1.65eV | 2g | 2g | 2g | 86.59g | 7.41g | 119.41 |