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From: ENGR 132 Team 13 (-30

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 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, its efficiency, and versatility. A few of the important constraints on the system are: the run time of the process, the data that is needed for input, and the ability of the deliverable to address the widely varying scenarios or alternate uses.

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 optimized.

**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, .

, where is the cost (or toxicity) 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 (Supplied in Memo 2). The second merely states that all the mass fractions should add up to a whole. The mathematical justification for this method can be found in the supporting materials.

In order to expand this method to multiple variables, we create a new variable called optimization attribute. This attribute is merely a weighted scaled sum of all the variables to optimize. For example, in this case cost and toxicity are both scaled so that they range from 0 to 100 and then are summed together assigning a weight based on user input. We then run a single attribute minimization on this new optimization attribute.

**Part 3, Results**

Using our model we have determined the various optimized methods to create 100g of product based on the supplied constraints are as follows: (In Cost/Toxicity Optimization we used a weighting factor of 1 i.e. cost is 1 times as important as toxicity. This can be changed by user input.)

**Demonstration A:** Band Gap Energy of Product: 1.33 eV, Materials used: 1-5

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Material | 1 | 2 | 3 | 4 | 5 | Cost | Toxicity |
| Cost | 2.00g | 2.00g | 61.14g | 2.00g | 32.86g | $2754.28 | 322.29 |
| Toxicity | 2.00g | 2.00g | 2.00g | 29.19g | 64.81g | $3321.87 | 176.81 |
| Cost/Toxicity | 2.00g | 2.00g | 2.00g | 29.19g | 64.81g | $3321.87 | 176.81 |

**Demonstration B:** Band Gap Energy of Product: 1.65, Materials used: 1-5 eV

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Material | 1 | 2 | 3 | 4 | 5 | Cost | Toxicity |
| Cost | 2.00g | 2.00g | 12.02g | 81.98g | 2.00g | $3799.68 | 144.06 |
| Toxicity | 2.00g | 2.00g | 2.00g | 86.59g | 7.41g | $3895.85 | 119.41 |
| Cost/Toxicity | 2.00g | 2.00g | 2.00g | 86.59g | 7.41g | $3895.85 | 119.41 |

**Demonstration C:** Band Gap Energy of Product: 1.33 eV, Materials used: 6-9

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Material | 6 | 7 | 8 | 9 | 10 | Cost | Toxicity |
| Cost | 2.00g | 2.00g | 69.32g | 2.00g | 24.68g | $2191.28 | 317.96 |
| Toxicity | 2.00g | 81.82g | 2.00g | 2.00g | 12.18g | $3757.90 | 195.82 |
| Cost/Toxicity | 2.00g | 81.82g | 2.00g | 2.00g | 12.18g | $3757.90 | 195.82 |

**Demonstration D:** Band Gap Energy of Product: 1.65 eV, Materials used: 6-9

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Material | 6 | 7 | 8 | 9 | 10 | Cost | Toxicity |
| Cost | 2.00g | 2.00g | 28.59g | 2.00g | 65.41g | $2028.36 | 195.77 |
| Toxicity | 2.00g | 33.53g | 2.00g | 2.00g | 60.47g | $2647.16 | 147.53 |
| Cost/Toxicity | 2.00g | 2.00g | 2.00g | 71.82g | 22.18g | $3458.02 | 255.64 |

**Demonstration E:** Band Gap Energy of Product: 1.33 eV, Materials used: 2,3,4,7,9

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Material | 2 | 3 | 4 | 7 | 9 | Cost | Toxicity |
| Cost | 77.78g | 16.22g | 2.00g | 2.00g | 2.00g | $3369.83 | 310.22 |
| Toxicity | 2.00g | 2.00g | 17.87g | 76.13g | 2.00g | $4036.13 | 190.13 |
| Cost/Toxicity | 2.00g | 2.00g | 17.87g | 76.13g | 2.00g | $4036.13 | 190.13 |

**Demonstration F:** Band Gap Energy of Product: 1.65 eV, Materials used: 2,3,4,7,9

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Material | 2 | 3 | 4 | 7 | 9 | Cost | Toxicity |
| Cost | 2.00g | 11.28g | 82.72g | 2.00g | 2.00g | $3822.79 | 143.84 |
| Toxicity | 2.00g | 2.00g | 86.04g | 7.96g | 2.00g | $3967.96 | 121.96 |
| Cost/Toxicity | 2.00g | 2.00g | 65.63g | 2.00g | 28.37g | $3962.00 | 168.74 |