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From: Team 18 - DMBP

Subject: Procedures for determining the cheapest and least toxic nanomaterial combinations

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**I. Introduction/Re-Usability:**

The direct user (the QD-PV fabrication team) needs a mathematical model that can determine the best configuration of particles to produce energy in the least toxic and/or the cheapest way. This model must not only output a solution based on varied inputs, but must also be easy to use or modify incase the fabrication team needs to make any changes. An algorithm with the ability to minimize toxicity while keeping the costs as low as possible will be considered successful, this should be paired with the fact that the model is easy to follow and make changes to. The constraints are the high number of variables, the multiple equations that need to be run and multiple sets of data that can complicate the process for finding the optimal solution. This algorithm must also use the previously given data about 10 QD materials and known equations.

The procedure is designed to use a mathematical model to optimize the fabrication team’s solution helping them to achieve their goal of reducing toxicity and costs to make this a commercial success. The key features are an easy to follow model that is flexible, helps the optimization process and has the ability to crunch large amounts of data to provide valuable results

The assumptions are that the quantum dots that are made will be produced without manufacturing errors and will be used in ideal situations without any random errors. We will ignore factors that would affect all materials equally such as interference from the environment like weather conditions that may reduce the efficiency of these QD cells. The limitations of our procedure are that it is still conceptual and theoretical. This means that the model is quite ideal and requires future real-world testing. Our mathematical model also assumes that the optimal combinations will be of only 2 materials. Although 5 materials are being tested at once, the minimum will most likely occur when the cheapest material and only one other material are combined.

**II. Procedure/Mathematical Model:**

Our mathematical model is in the form of a matlab .m file as attached. The steps that this program takes are as follows:

Procedural steps to determine minimum cost (ignore toxicity) are:

Inputs: Which of the 5 materials are being used, desired energy, decimal accuracy (assumed 2 decimals for the rest of this procedure)

Error messages: If values above 1.82 or below 1.19 are given, it will return an error as those are not possible to create with the given materials (regardless of toxicity/cost)

1. Calculate the band gap energy of each of the 10 given nanomaterials.

2. Choose any material

3. Set this material’s mass percentage to maximum (92) and the others to their minimum (2)

4. Calculate the effective band gap energy of this material combination.

5. If the effective band gap energy of this material is equal to the desired, do not change the mass percentages

6. If the effective band gap energy is different, then choose any of the remaining materials.

7. Subtract .01% from the original material (set to 92 originally)

8. Add .01% of the other material to the current combination (for example: it should be 2, 2, 2, 2.01, and 91.99% at this point)

9. Calculate the effective band gap energy of the current mixture

10. Continue this process until either the original material (originally 92) hits 2% or the effective band gap energy is equal to the desired band gap energy

11. Save this final combination for these two materials to be used later

12. Select another material and repeat steps 6 – 11

13. Once all possible material combinations have been tried (9 steps) calculate the cost of each combination.

14. Select the combination of the lowest cost and print its mixture

15. Also, print the effective band gap energy, toxicity, and number of iterations taken to make that ideal mixture

Procedural steps to determine minimum toxicity:

1. This procedure is identical to that of the min. cost except for in all calculations costs are replaced by toxicities. i.e. Determine which material has the lowest toxicity instead of which is cheapest

Procedural steps for minimizing both:

1. Once again, the procedure is very similar. However, here, instead of determining lowest cost or lowest toxicity, the program determines the lowest “Cost – Toxicity combination”

2. We define the cost – toxicity combination is defined as the following:

Where “Avg” are the average value for ea. material. For example, Avg cost = avrg(45, 35, 25, 40, 30, 30, 41, 22, 40, 18) = $32.6/g . Using this definition, we are able to find which materials are good at not just being low cost or toxicity but both. Materials with these properties would be ideal as a balance between profit and health/environmental friendliness.

The rationale for our model’s critical steps of setting a material to 92g are based on the fact that the cheapest possible combinations are going to come from a combination of the cheapest material or and (likely) materials with a low cost/energy ratio. By making the majority of the mixture those and not other more expensive materials, we minimize costs. The same goes for low toxicity materials also being set to 92g. (out of 100g)

This problem is extremely complex due to the large number of variables which are trying to be maximized. With fewer variables, one could determine the exact optimal solution in closed form and simply plug the variables into that equation and have it output the best solution. However, here this is not possible. Instead, our mathematical model does not find the exact answer, only an answer that is so close to the true value that within any practical rounding, it is identical. It does this through many steps but eventually gets there and is able to handle the large number of variables and output solutions to as many degrees of accuracy as necessary.

**III. Results (Share-ability):**

On the following pages are a few demonstrations of the results of our algorithm. They have been tested for a variety of desired energies and possible mixable materials.

Demonstration A: Goal - (*Eg,quantum dot*)*eff* = 1.33 eV

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | Scenario 1: Min cost | | Scenario 2: Min Toxicity | | Scenario 3: Min both | |
| Material |  | (*Eg,quantum dot*)*eff* | Material QTY | (*Eg,quantum dot*)*eff* | Material QTY | (*Eg,quantum dot*)*eff* |
| QD1 | 2 | 1.7972 | 25.29 | 1.7972 | 25.29 | 1.7972 |
| QD2 | 2 | 1.3009 | 2 | 1.3009 | 2 | 1.3009 |
| QD3 | 61.18 | 1.4023 | 2 | 1.4023 | 2 | 1.4023 |
| QD4 | 2 | 1.7035 | 2 | 1.7035 | 2 | 1.7035 |
| QD5 | 32.82 | 1.1460 | 68.71 | 1.1460 | 68.71 | 1.1460 |
| Iterations:  54807 |  |  |  |  |  | T |
| 27.54 | 322.36 | 33.99 | 204.00 | 33.99 | 204.00 |

Demonstration B: Goal - (*Eg,quantum dot*)*eff* = 1.65 eV

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | Scenario 1: Min cost | | Scenario 2: Min Toxicity | | Scenario 3: Min both | |
| Material | Material QTY | (*Eg,quantum dot*)*eff* | Material QTY | (*Eg,quantum dot*)*eff* | Material QTY | (*Eg,quantum dot*)*eff* |
| QD1 | 2 | 1.7972 | 2 | 1.7972 | 2 | 1.7972 |
| QD2 | 2 | 1.3009 | 9.52 | 1.3009 | 9.52 | 1.3009 |
| QD3 | 12.05 | 1.4023 | 2 | 1.4023 | 2 | 1.4023 |
| QD4 | 81.95 | 1.7035 | 84.48 | 1.7035 | 84.48 | 1.7035 |
| QD5 | 2 | 1.1460 | 2 | 1.1460 | 2 | 1.1460 |
| Iterations:  56305 | Cost ($/g) | Toxicity | Cost ($/g) | Toxicity | Cost ($/g) | Toxicity |
| 37.99 | 144.15 | 39.12 | 129.04 | 39.12 | 129.04 |

Demonstration C: Goal - (*Eg,quantum dot*)*eff* = 1.33 eV

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | Scenario 1: Min cost | | Scenario 2: Min Toxicity | | Scenario 3: Min both | |
| Material | Material QTY | (*Eg,quantum dot*)*eff* | Material QTY | (*Eg,quantum dot*)*eff* | Material QTY | (*Eg,quantum dot*)*eff* |
| QD6 | 2 | 1.7522 | 2 | 1.7522 | 2 | 1.7522 |
| QD7 | 2 | 1.2341 | 81.83 | 1.2341 | 81.83 | 1.2341 |
| QD8 | 69.32 | 1.1111 | 2 | 1.1111 | 2 | 1.1111 |
| QD9 | 2 | 1.5975 | 2 | 1.5975 | 2 | 1.5975 |
| QD10 | 24.68 | 1.8968 | 12.17 | 1.8968 | 12.17 | 1.8968 |
| Iterations:  43498 | Cost ($/g) | Toxicity | Cost ($/g) | Toxicity | Cost ($/g) | Toxicity |
| 21.91 | 317.96 | 37.58 | 195.83 | 37.58 | 195.83 |

Demonstration D: Goal - (*Eg,quantum dot*)*eff* = 1.65 eV

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | Scenario 1: Min cost | | Scenario 2: Min Toxicity | | Scenario 3: Min both | |
| Material | Material QTY | (*Eg,quantum dot*)*eff* | Material QTY | (*Eg,quantum dot*)*eff* | Material QTY | (*Eg,quantum dot*)*eff* |
| QD6 | 2 | 1.7522 | 2 | 1.7522 | 2 | 1.7522 |
| QD7 | 2 | 1.2341 | 33.54 | 1.2341 | 33.54 | 1.2341 |
| QD8 | 28.6 | 1.1111 | 2 | 1.1111 | 2 | 1.1111 |
| QD9 | 2 | 1.5975 | 2 | 1.5975 | 2 | 1.5975 |
| QD10 | 65.4 | 1.8968 | 60.46 | 1.8968 | 60.46 | 1.8968 |
| Iterations:  54795 | Cost ($/g) | Toxicity | Cost ($/g) | Toxicity | Cost ($/g) | Toxicity |
| 20.28 | 195.80 | 26.47 | 147.54 | 26.47 | 147.54 |

Demonstration E: Goal - (*Eg,quantum dot*)*eff* = 1.33 eV

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | Scenario 1: Min cost | | Scenario 2: Min Toxicity | | Scenario 3: Min both | |
| Material | Material QTY | (*Eg,quantum dot*)*eff* | Material QTY | (*Eg,quantum dot*)*eff* | Material QTY | (*Eg,quantum dot*)*eff* |
| QD2 | 2 | 1.3009 | 2 | 1.3009 | 2 | 1.3009 |
| QD3 | 46.36 | 1.4023 | 2 | 1.4023 | 2 | 1.4023 |
| QD4 | 2 | 1.7035 | 17.89 | 1.7035 | 17.89 | 1.7035 |
| QD7 | 47.64 | 1.2341 | 76.11 | 1.2341 | 76.11 | 1.2341 |
| QD9 | 2 | 1.5975 | 2 | 1.5975 | 2 | 1.5975 |
| Iterations:  49870 | Cost ($/g) | Toxicity | Cost ($/g) | Toxicity | Cost ($/g) | Toxicity |
| 33.42 | 294.72 | 40.36 | 190.11 | 40.36 | 190.11 |

Demonstration F: Goal - (*Eg,quantum dot*)*eff* = 1.65 eV

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | Scenario 1: Min cost | | Scenario 2: Min Toxicity | | Scenario 3: Min both | |
| Material | Material QTY | (*Eg,quantum dot*)*eff* | Material QTY | (*Eg,quantum dot*)*eff* | Material QTY | (*Eg,quantum dot*)*eff* |
| QD2 | 2 | 1.3009 | 2 | 1.3009 | 2 | 1.3009 |
| QD3 | 2 | 1.4023 | 2 | 1.4023 | 2 | 1.4023 |
| QD3 | 65.72 | 1.7035 | 86.06 | 1.7035 | 86.06 | 1.7035 |
| QD7 | 2 | 1.2341 | 2 | 1.2341 | 2 | 1.2341 |
| QD9 | 28.28 | 1.5975 | 28.28 | 1.5975 | 28.28 | 1.5975 |
| Iterations:  66222 | Cost ($/g) | Toxicity | Cost ($/g) | Toxicity | Cost ($/g) | Toxicity |
| 39.62 | 168.56 | 39.68 | 121.94 | 39.68 | 121.94 |

Thank you for the opportunity to help you optimize this new technology that can potentially change the world of energy production ad consumptions. We hope these procedures help the fabrication team to reduce both toxicity and costs of your products.

Sincerely,

Team 18