To: Teresa Wall, Vice President of Research, Power-By-Nano Technologies

From: Team 13

Subject: Procedure for band gap energy optimization

Date: February 19, 2015

**I. Introduction/Re-Usability**

Our team was asked to develop an optimization algorithm. The direct user is the QD-PV fabrication team. The direct user needs our algorithm that provides a simple way to minimize either the cost and/or the toxicity of the ‘recipe’ for a given goal Quantum Dot (QD) band gap energy. The criteria for success of our optimization algorithm are successful minimization, robustness (accepts variety of inputs/volumes and provides appropriate outputs), and ease of use. The constraints are the attributes of the materials including their cost and toxicity.

The procedure is designed to minimize the cost and/or toxicity of the product. The key features are selection of the best materials to use, adding all materials to meet minimum usage requirements, and creating a final ‘recipe.’

The assumptions are that there are no free materials being use (cost/toxicity must be greater than zero). The limitations of our procedure are the amount of data that can be entered into the function is bounded by the capabilities of the platform used, and logical contradictions (the goal being impossible to meet using given materials).

**II. Procedure/Mathematical Model**

The procedural steps to create an ‘optimization attribute’ are:

1. Assign relative importance to each attribute that you wish to minimize (e.g. if toxicity is twice as important as cost, toxicity will be assigned a value of 2 and cost will be assigned 1).

2. Multiply each attribute by its relative importance and then divide by the maximum value of that attribute. Call this the scaled attribute value. (e.g. if cost has a relative importance of 1 and its maximum value is 50, then a cost of 25 would be scaled to 1\* (25 / 50) or 0.5).

3. Sum all the scaled attribute values for each material. (e.g. if a material has a scaled cost of 0.5 and a scaled toxicity of 0.2 its optimization attribute is 0.7).

The procedural steps to assign a ‘value’ to each material are:

1. Find the QD band gap energy for each material using the equation provided in memo 1.

2. Find the absolute value of the difference between the goal band gap energy and each QD material’s band gap energy.

3. Divide the difference by the ‘optimization attribute.’ This is the ‘value’ of the material.

The procedural steps to find the optimal ‘recipe’ are:

1. Select the most valuable material with QD band gap energy over the goal band gap energy, call this material ‘o.’

2. Select the most valuable material with QD band gap energy under the goal band gap energy, call this material ‘u.’

3. Solve the following system of equations:

Where is goal band gap energy; and are the band gap energies of ‘o’ and ‘u’, and are the mass fraction of ‘o’ and ‘u’ (in addition to 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.

4. To get the amount of ‘o’ necessary add xo to xmin and multiply this sum by the total needed mass. The same process is followed for ‘u.’

5. For all materials that are not ‘o’ or ‘u’ use only the minimum allowed amount. (xmin \* total required)

The rationale for our model’s critical steps of creating an ‘optimization attribute’ are based on the fact that multiple attributes need to be put on the same scale (level the playing field) in order to be compared (hence the creation of the scaled attribute value). As scaled attribute value also takes into account each attribute’s relative importance to the user. Summing these together gives you a combined optimization attribute that can then be minimized by the procedure above.

The rationale for our model’s critical steps of creating a ‘value’ are based on the fact that the materials that most affect the goal band gap energy are the ‘farthest’ from that goal. This is derived from the way averages work. When maximizing this it is also important to minimize cost and therefore the value and the cost must have an inverse relationship.

The rationale for our model’s critical steps of creating a ‘recipe’ are based on the equation provided in memo 2 (for finding the band gap energy of a mixture of materials). Mass fractions must add up to the whole.

Our team has identified the complexity of this problem as the need to minimize multiple attributes at the same time and accept many materials. Our mathematical model addresses the problem’s complexity by allowing for as many materials and optimization attributes as the user desires and hardware/software permits.

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

**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 |

**Demonstration E:** Band Gap Energy of Product: 1.33 eV, Materials used: 2,3,4,7,9,11,12

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Material | 2 | 3 | 4 | 7 | 9 | 11 | 12 | Cost | Toxicity |
| Cost | 2.00g | 2.00g | 2.00g | 2.00g | 2.00g | 67.49g | 22.51g | $7133.96 | 723.45 |
| Toxicity | 2.00g | 2.00g | 85.33g | 2.00g | 2.00g | 2.00g | 4.67g | $3899.71 | 134.00 |
| Cost/Toxicity | 2.00g | 2.00g | 2.00g | 2.00g | 2.00g | 67.49g | 22.51g | $7133.96 | 723.45 |

**Demonstration F:** Band Gap Energy of Product: 1.65 eV, Materials used: 2,3,4,7,9,11,12

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Material | 2 | 3 | 4 | 7 | 9 | 11 | 12 | Cost | Toxicity |
| Cost | 2.00 | 2.00 | 2.00 | 2.00 | 2.00 | 67.49 | 22.51 | 7133.96 | 723.45 |
| Toxicity | 2.00 | 2.00 | 85.33 | 2.00 | 2.00 | 2.00 | 4.67 | 3899.71 | 134.00 |
| Cost/Toxicity | 2.00 | 2.00 | 2.00 | 2.00 | 2.00 | 67.49 | 22.51 | 7133.96 | 723.45 |

**IV. Other Information:**

Materials 11 and 12 are as follows

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Material | Bulk Band Gap Energy | Dielectric Constant | Quantum Dot Radius | Cost | Toxicity |
| 11 | 2 | 3.4 | 5.6 | 100 | 10 |
| 12 | 1.11 | 5.0 | 3.9 | 1 | 1 |

Both these materials test the reasonable extremes of the attribute values.

Thank you for the opportunity to work with you on this unique mathematical problem. We hope these procedures help the fabrication team to create a product that is both inexpensive and environmentally responsible.

Sincerely,

Team 13,

Apoorva Kharche

Broderick Schwartz

Rashid Sarwar

Yash Shah