**Supporting Information**

**A Data-Driven Framework for Prediction of Carbon Based Hybrid Catalyst Layer Performance in Polymer Electrolyte Fuel Cells using Artificial Neural Networks**

All available experimental data with different cathode types based on carbon materials were gathered in Table S1. Literatures that had complete information about cathode materials such as total surface area, Pt catalyst percentage, voltammetry diagrams as well as current density-voltage-power density diagrams were marked with an asterisk in Table S1. These data have been used in the final programming.

**Table S1.**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Number** | **Cathode material** | **size of Pt particles (nm)** | **Pt content (wt%)** | **Pt surface area (m2/g)** | **Pt-Free cathode surface area (m2/g)** | **Cathode general surface area (m2/g)** | **ECSA (m2/g)** |
| 1\* [1] | Pt/CB (HE00) | 2 | 30 | - | - | - | 50 |
| Pt/rGO-CB (HE25) | 1.7 | 30 | - | - | - | 55 |
| Pt/rGO-CB (HE50) | 1.7 | 30 | - | - | - | 49 |
| Pt/rGO-CB (HE75) | 1.7 | 30 | - | - | - | 45 |
| Pt/rGO (HE100) | 1.3 | 30 | - | - | - | 65 |
| 2 [2] | Vulcan-Pt | 3.1 | 45 | - | - | - | 59.5 |
| Pt-Vulcan-PBI (Polybenzimidazole) | 3.1 | 44.8 | - | - | - | 70.5 |
| 3 [3] | MPC22 (Mesoporous carbon sphere synthesized by 22 nm colloidal silica) | 22 | - | - | 1020 | - | - |
| 4 [4] | Pt-CNC (carbon nano coil) | 4.7 | 20 | - | 124 | - | - |
| Pt-Vulcan | 3.2 | 20 | - | 218 | - | - |
| Pt-C | 3 | 20 | - | - | - | - |
| 5\* [5] | GNP-CB-Pt (H50) | 1.85 | 16.3 | 24.6456 | 397 | 356.9346 | 45.58 |
| GNP-CB-Pt (H60) | 2.1 | 18.2 | 24.2424 | 485 | 420.9724 | 48.13 |
| GNP-CB-Pt (H70) | 2.04 | 19.2 | 26.3266 | 485 | 418.2066 | 44.73 |
| GNP-CB-Pt (H80) | 1.84 | 21.2 | 32.2286 | 505 | 430.1686 | 52.24 |
| GNP-CB-Pt (H90) | 2.05 | 22.5 | 30.701 | 650 | 534.451 | 45.75 |
| GNP-Pt (H100) | 1.7 | 22.8 | 37.5154 | 759 | 623.4634 | 49.66 |
| 6 [6] | CNF-Pt (carbon nano fiber LT-F) | 5.4 | 19.9 | - | 185 | - | - |
| Vulcan-Pt | - | - | - | 218.4 | - | - |
| 7 [7] | Pt/SWCNT (single-wall carbon nano tubes) | 11 | 20 | - | - | - | - |
| Ru/SWCNT | - | 20 | - | - | - | - |
| MO/SWCNT | - | 20 | - | - | - | - |
| Pt-MO(50)/SWCNT | - | 40 | - | - | - | - |
| Pt-MO(33)/SWCNT | 13 | 30 | - | - | - | - |
| Pt-MO(20)/SWCNT | - | 25 | - | - | - | - |
| Pt-Ru(20)/SWCNT | 10 | 25 | - | - | - | - |
| Pt-Ru(33)/SWCNT | - | 30 | - | - | - | - |
| Pt-Ru(50)/SWCNT | - | 40 | - | - | - | - |
| 8 [8] | Pt/C | - | 40 | - | - | 93.2 | 67 |
| Pt/MWCNT1 | 2.7 | 30 | - | - | 103.6 | 50 |
| Pt/MWCNT2 | 4.4 | 42 | - | - | 63.6 | 48 |
| Pt/MWCNT3 | 2.3 | 26 | - | - | 121.6 | 37 |
| Pt/MWCNT4 | 2.4 | 29 | - | - | 116.6 | 42 |
| Pt/MWCNT5 | 4.2 | 34 | - | - | 66.6 | 25 |

**Table S1 (continued)**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Number** | **Cathode material** | **size of Pt particles (nm)** | **Pt content (wt%)** | **Pt surface area (m2/g)** | **Pt-Free cathode surface area (m2/g)** | **Cathode general surface area (m2/g)** | **ECSA (m2/g)** |
| 9 [9] | Pt-GO | - | 40 | - | - | - | 13.62 |
| Pt-GO-CeO2 6% | - | 40 | - | - | - | 43.3 |
| Pt-GO-CeO2 8% | - | 40 | - | - | - | 52.46 |
| Pt-GO-CeO2 10% | - | 40 | - | - | - | 49.07 |
| Pt-GO-CeO2 15% | - | 40 | - | - | - | 34.23 |
| 10 [10] | Pt-Gr-C | 7.7 | 15 | - | - | - | 79 |
| Pt-C | 3.3 | 15.6 | - | - | - | 98 |
| 11 [11] | Pt/NRGO | 2.5 | 20 | - | - | - | 75.6 |
| Pt/GO | 2.8 | 20 | - | - | - | 64.8 |
| Pt/C | 3.2 | 20 | - | - | - | 53.3 |
| 12 [12] | Pt-C | - | - | - | - | - | 19 |
| Pt-Gr | 2.4 | - | - | - | - | 18.5 |
| Pt-B-Gr | 2.37 | 39 | - | - | - | 21.4 |
| Pt-B-Gr/CB0.2 | - | - | - | - | - | 30.3 |
| Pt-B-Gr/CB0.3 | - | - | - | - | - | 33.6 |
| Pt-B-Gr/CB0.4 | - | - | - | - | - | 29.6 |
| 13 [13] | Pt-Gr (dry) | 3.5 | 40 | - | - | 862 | - |
| Gr (dry) | - | - | - | - | 44 | - |
| 14 [14] | NG180 | 3.3 | - | - | - | 179.8 | 36 |
| NGA800 | 3.5 | - | - | - | 208.6 | 32 |
| 15\* [15] | rGO-Pt (H100) | 2.9 | 25.2 | 24.3067 | 41 | 54.9742 | 60 |
| rGO-CB-Pt (H90) | 2.6 | 16.2 | 17.4287 | 57 | 65.1937 | 67 |
| rGO-CB-Pt (H80) | 2.3 | 18.4 | 22.3776 | 73 | 81.9454 | 42 |
| rGO-CB-Pt (H70) | 1.9 | 18.7 | 27.5303 | 87 | 98.2587 | 67 |
| rGO-CB-Pt (H60) | 2.6 | 21.4 | 23.0231 | 105 | 105.5516 | 61 |
| rGO-CB-Pt (H50) | 2.4 | 15 | 17.4825 | 122 | 121.1825 | 56 |
| CB-Pt (H00) | 2.4 | 6 | 6.9929 | 208 | 202.5125 | 65.7 |
| 16\* [16] | Pt | 3 | 100 | 66 | 66 | 66 | 13 |
| CB-Pt | 3 | 50 | 46.6186 | 208 | 150.6186 | 19 |
| GO-Pt (50-50) | 3.3 | 50 | - | - | - | 16.9 |
| 17 [17] | Pt-CB | 3.7 | 45 | - | - | - | 42 |
| Pt-SWCNT | 3.5 | 33 | - | - | - | 31 |
| Pt-MWCNT | 2.6 | 63 | - | 50,60 | - | 66 |
| Pt-G | 3.2 | 23 | - | - | - | 22 |
| 18 [18] | Pt/C | 2.6 | 20 | - | - | - | - |
| DPC (Nitrogen and sulfur co-doped porous carbon) | 2.6 | 19.54 | - | - | - | - |
| Pt/DPC | 2.6 | 19.54 | - | - | - | - |
| \* Articles used in the final classification. | | | | | | | |

The accuracy of ANN model was examined by computing MSE, R, Bias and weight matrices versus various neurons number for the first and second modeling. Results of Bias and weight matrices are shown in Table S2-S4.

**Table S2. Bias matrix in the first and second modeling**

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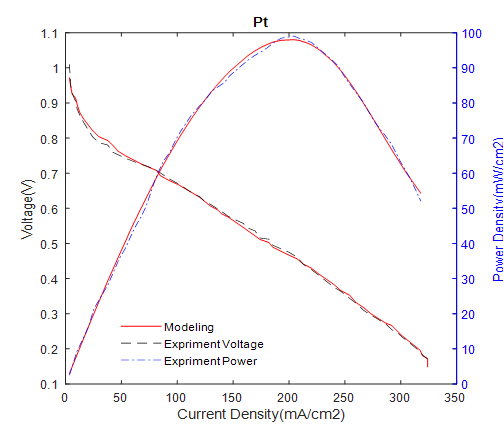
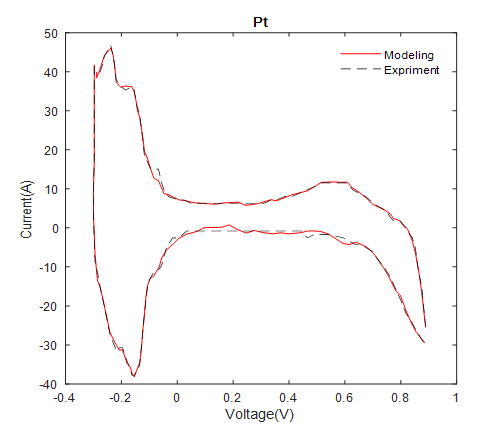
**Table S3. Weight matrix in hidden layer for the first and second modeling**

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**Table S4. Weight matrix in output layer for the first and second modeling**

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Figures S3-S6 show a comparison between cyclic voltammetry and current density-voltage-power density experimental data and the values obtained from the modeling for the training data.



**(a)**

**(b)**

|  |  |  |  |
| --- | --- | --- | --- |
|  | |  |  |
|  | **Figure S1. (a) Cyclic voltammetry and (b) current density-voltage-power density diagrams with training data for pure Pt.** | | |

**(b)**

**(a)**

**Figure S2. (a) Cyclic voltammetry and (b) current density-voltage-power density diagrams with training data for rGO-CB cathodes with different ratios.**

**(b)**

**(a)**

**(a)**

**Figure S3. (a) Cyclic voltammetry and (b) current density-voltage-power density diagrams with training data for CB-Pt cathodes with different ratios.**

**(a)**

**(b)**

**Figure S4. (a) Cyclic voltammetry and (b) current density-voltage-power density diagrams with training data for GNP-CB with different ratios.**

The graphs of validation data for cyclic voltammetry and current density-voltage-power density are shown in Figures S5-S8.

**(b)**

**(a)**

**Figure S5. (a) Cyclic voltammetry and (b) current density-voltage-power density diagrams with validation data for pure Pt.**

**(b)**

**(a)**

**Figure S6. (a) Cyclic voltammetry and (b) current density-voltage-power density diagrams with validation data for rGO-CB cathodes with different ratios.**

**(b)**

**(a)**

**Figure S7. (a) Cyclic voltammetry and (b) current density-voltage-power density diagrams with validation data for CB-Pt cathodes with different ratios.**

**(b)**

**(a)**

**Figure S8. (a) Cyclic voltammetry and (b) current density-voltage-power density diagrams with validation data for GNP-CB cathodes with different ratios.**

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