**Physicochemical parameter influences and their optimization on the biosynthesis of MnO2 nanoparticles using *Vernonia amygdalina* leaf extract**

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**Table S1** RSM model fit summary for MnO2 maximum absorption at 320 nm.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Source** | **Sequential p-value** | **Lack of Fit p-value** | **Adjusted R²** | **Predicted R²** |  |
| Linear | < 0.0001 | 0.0265 | 0.8454 | 0.8008 |  |
| 2FI | 0.5632 | 0.0225 | 0.8373 | 0.5555 |  |
| **Quadratic** | **0.0026** | **0.1059** | **0.9496** | **0.8452** | **Suggested** |
| Cubic | 0.1059 |  | 0.9868 |  | Aliased |

**Table S2** The calculated crystallite size of as synthesized γ-MnOOH and α-MnO2 NPs (calcined at 450oC).

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Precursor | Reducing agent | Sample type | d-spacing (nm) | 2θ (degree) | FWHM (degree) | Miller indices (hkl) | Crystallite size (nm) |
| KMnO4 | *Vernonia amygdalina* | As synthesized γ-MnOOH | 0.34085  0.22593  0.16712 | 26.036  37.155  54.806 | 0.4009  0.5082  0.5516 | 1 1 -1  2 0 0  3 1 -1 | 21.25  17.23  16.95  Average = 18.47 |
| α-MnO2 (2 hour calcination) | 0.69569  0.24623 | 12.971  35.917 | 0.3757  0.3811 | 1 1 0  4 0 0 | 22.24  22.90  Average = 22.57 |
| α-MnO2 (3 hour calcination) | 0.69792  0.35008  0.23830 | 12.479  25.228  37.218 | 0.3875  0.4050  0.4453 | 1 1 0  2 2 0  2 1 1 | 21.55  21.00  19.67  Average = 20.74 |

FWHM = Full width at maximum at half maximum

**Table S3** Grain structure summary of MnO2 NPs calcined at 450 oC.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Sample | Calcination time (hour) | Method | Number of grain | Plane grain (%) | Mean grain size (nm) | Mean grain area (nm2) | Laplace grain volume (µm3) |
| MnO2 NPs | 2 | Threshold | 1767 | 58.646 | 33.6118 | 67886.3 | 2.43937 |
| Watershed | 3822 | 0.759 | 17.8796 | 406.352 | 1935.944 |
| 3 | Threshold | 587 | 67.276 | 55.5108 | 225948 | 3.29340 |
| Watershed | 3929 | 2.157 | 22.2123 | 1082.13 | 6905.321 |

**Table S4** Inverted height distribution parameters of MnO2 NPs calcined at 450 oC.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Sample | Calcination time (hour) | Method | Ra (µm-1) | Rq (µm-1) | Rsk | Rku | Area under curve |
| MnO2 NPs | 2 | Threshold | 13.6980 | 15.8247 | 1.07324 | 0.460877 | 0.986495 |
| Watershed | 5.59037 | 6.52990 | 0.752972 | -0.511681 | 0.994143 |
| 3 | Threshold | 9.00009 | 9.62247 | -0.308431 | -1.63821 | 0.988878 |
| Watershed | 6.09652 | 7.16758 | 0.617925 | -0.614967 | 0.998252 |