**Polymer Grafting of Graphene Oxide through Esterification of Terephthalic Acid and Allyl Alcohol for Metronidazole Drug Delivery:** **Central Composite Design Optimization Study**

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The following is included as additional **Supporting Information** for this paper:

**Figure Captions:**

**Fig. S1.** TGA thermogram of GO/TPAA cl-poly (AA)/TPA.

**Fig. S2.** XRD pattern of GO/TPAA cl-poly (AA)/TPA.

**Fig. S3.** FT-IR spectra of GO/TPAA (a) and GO/TPAA cl-poly (AA)/TPA (b).

**Fig. S4.** N2 adsorption–desorption isotherm of GO/TPAA cl-poly (AA)/TPA.

**Fig. S5.** plot of ln (KL) versus 1/T.

**Fig. S6.** Influence of reusability on MNZ adsorption.

**Table captions:**

**Table S1.** Isotherm model parameters for the adsorption of MNZ onto GO/TPAA cl-poly (AA)/TPA.

**Table S2.** Kinetic model parameters for the adsorption of MNZ onto GO/TPAA cl-poly (AA)/TPA.

**Table S3.** Thermodynamics parameters for the adsorption of MNZ onto GO/TPAA cl-poly (AA)/TPA.

**Table S4.** Results of the correlation coefficients and rate constants of different models for release curve of MNZ from GO/TPAA cl-poly (AA)/TPA (pH=1.2 and 7.4).



**Fig. S1**

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 **Fig. S2**





**Fig. S3**



**Fig. S4**



 **Fig. S5**

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**Fig. S6**

**Table S1**

|  |  |  |
| --- | --- | --- |
| **Model** | **Parameter**  **T=298.15K** | **Value** **T= 308.15 K T= 323**.**15K**  |
| **Langmuir** | qm (mg g-1)kl (L mg-1)RlR2 | 7.7760.0240.2870.9956 | 10.5820.0430.1860.9932 | 11.0980.1090.0830.9913 |
| **Ferundlich** | nLn(kf)kf(mg11/nL1/ng-1)R2 | 1. 508-1.0880.3360.9947 | 1.594-0.320.7260.9836 | 1.6920.3011.3510.9885 |
| **Temkine** | BAT (L mg-1)R2 | 1.2950.4190.9515 | 2.2270.4690.9945 | 2.4331.0610.9828 |
| **Dubinin-Radushkevich** | Kad (mol2 kJ-2)Ln (qs)qs (mg g-1)R2 | 0.000021.3443.8340.8863 | 0.0000071.7355.6720.9141 | 0.0000021.9016.6940.8406 |

**Table S2**

|  |  |  |
| --- | --- | --- |
| **Model** | **Parameter** |  **Value** |
| **Pseudo-first-order model** | qe (mg g-1)K1 (min-1)R2 | 4.0730.00390.9486 |
| **Pseudo-second-order model** | qe (mg g-1)K2 (g mg-1min-1)R2 | 1.6941.7790.9999 |
| **Intra-particle diffusion** | Ki (g mg-1min-1/2)Ci (mg g-1)R2 | 0.0811.3650.9419 |

**Table S3**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Sample** | **Temperature (K)** | **ΔHo (J mol-1)** | **ΔSo (J mol-1 K-1)** | **ΔGo (J mol-1)** |
| **GO/TPAA cl-poly (AA)/TPA** | 298.15308.15323.15 | 47637.56 | 186.2918 | $-$7.905$-$9.768$-$12.562 |

**Table S4**

|  |  |  |  |
| --- | --- | --- | --- |
| **Zero order**pH=1.2 pH=7.4 | **First order**pH=1.2 pH=7.4 | **Higuchi** pH=1.2 pH=7.4 | **Korsmeyer – Peppas**pH=1.2 pH=7.4 |
| **K0  R2 K0  R2** | **K1  R2 K1 R2** | **KH  R2 KH  R2** | **n KKP  R2 KKP  R2** |
| 5.226 0.9919 5.362 0983 | 0.151 0.9562 0.255 0.9863 | 34.579 0.9871 34.03 0.9286 | 0.5 34.077 0.9889 34.03 0.92860.6 26.015 0.9937 26.132 0.94410.7 20.318 0.9962 20.525 0.95710.8 16.118 0.9966 16.37 0.96790.9 12.928 0.9951 13.198 0.97651 10.454 0.9919 10.724 0.9830  |