**Supporting Information**

**MIL-101 (Cr) Hybrid Nanoporous Carbon Derived MOF as a Nano-adsorbent for Dye Removal Using RSM-CCD**

Soheila Sharafinia1, Alimorad Rashidi2\*

1Department of chemistry, Faculty of Science, Shahid Chamran University of Ahvaz, Ahvaz, Iran

2\*Nanotechnology Research Center, Research Institute of Petroleum Industry (RIPI), Tehran, Iran

Corresponding author.

E-mail addresses: 2\*rashidiam@ripi.ir

Table S1: The linear form of the isotherms.

|  |  |  |
| --- | --- | --- |
| **Isotherms Name** | **Linear Form** | **Parameters** |
| Langmuir |   | qm (mg. g-1) = Maximum adsorption capacity KL (L. mg−1)= Langmuir adsorption constant |
| Freundlich |  | n= The intensity adsorptionKF= The adsorption capacity |
| Tamkin | B1 =  | B1 (J. mol-1) and KT (L. g-1)=Temkin constantsb= The heat of adsorptionk= The maximum bond energy |
| D-R |  | β (KJ2.mmol-2) = The coefficient of mean free adsorptionε (J. mmol-1)= Polanyi potentialE (KJ. mmol-1)= Amount of energy |

Table S2: Isotherm constant and correlation coefficients calculated for MB adsorption by Zn-MOF-5 NPC@MIL nanohybrid.

|  |
| --- |
| Freundlich |
| **Parameter** | n | Log KF | R2 |
|  | 1.6 | 5.98 | 0.95 |
| **Langmuir** |
| **Parameter** | Qm (mg.g-1) | KL (L.mg-1) | R2 |
|  | 1000 | 0.714 | 0.99 |
| **Temkin** |
| **Parameter** | B1 | KT(L.mg-1) | R2 |
|  | 411 | 2.94 | 0.98 |
| **D-R** |
| **Parameter** | β\*10-3(KJ2.mmol- 2) | qm (mg.g-1) | E\*10-3(KJ. mmol-1) | R2 |
|  | 0.052 | 473.42 | 3.53 | 0.97 |

Table S3: Linear form of each kinetic models.

|  |  |  |  |
| --- | --- | --- | --- |
| **Eq.** | **Linear Form** | **Parameters** |  |
| **PFO** |  | qt (mg. g-1) =Adsorption capacity at time (t)qe (mg. g-1) = Adsorption capacity at equilibriumk1(min−1) = The PFO rate constant |  |
| **PSO** |  | K2 (g. mg-1. min)= The rate constant of the PSO. |  |
| **Elovich** | ln (t) |  = The initial phenol adsorption rate (g.mg-1) = The surface coverage |  |
| **Intraparticle Diffusion** |  | C (mg. g-1) =a constant of the model |  |

Table S4: Adsorption kinetic parameters for MB removal onto Zn-MOF-5 NPC@MIL nanohybrid.

|  |
| --- |
| **PFO** |
| Parameter | R2 | K1 (min-1) | qe, Calc (mg.g-1) |
|  | 0.98 | 0.017 | 13.80 |
| **PSO** |
| Parameter | R2 | K2 (min-1) | qe, Calc (mg.g-1) |
|  | 1 | 0.018 | 83.33 |
| **Elovich** |
| Parameter | R2 | (mg.g-1·min-1) | (mg.g-1) |
|  | 0.96 | 7.07E+08 | 0.29 |
| **Intraparticle** |
| Parameter |  | R2 | Kdif (L/min) | C |
|  | Step (1) | 0.99 | 2.4 | 65 |
|  | Step (2) | 0.99 | 0.81 | 73 |
|  | Step (3) | 0.2 | -0.026 | 78 |
| **qe, Exp (mg. g-1)** |  | 78.55 |  |