**Supplementary Material**

**Novel grafted hydrogel for Iron and ammonia removal from ground water, synthesis and computational chemistry study**

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**Figure S1: Effect Temperature on the removal iron(A) and ammonia(b) efficiency at different dose of grafted hydrogel. Van’t Hoff plot for the adsorption of iron (c) and ammonia (d) on grafted hydrogel**



**Figure S2: Temkin isotherm for iron (a) and ammonia (b) removal by grafted hydrogel**



**Figure S3: Pseudo‑first‑order kinetic model of iron (a) and ammonia (b) removal. Pseudo‑second‑order kinetic model of iron (c) and ammonia (d) removal.**

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**Figure S4: The optimized structure of complexed grafted hydrogel different positions with NH4+ ion at B3LYP/6-311G(d,p) level of theory**

**Table S1: IR bands and their assignments for hydrogel and grafted hydrogel.**

|  |  |  |  |
| --- | --- | --- | --- |
| **Wave number cm-1** | **Wave number cm-1** | **Assignments** | **Ref.** |
| **Hydrogel** | **Grafted hydrogel** |
| 612**vw** | 608**m** | Stretching vibration of substituted benzene ring | a\*  |
| 777**vw** | 783**s** |
| 1115w | 1110w | C-O and C-N stretching  | b\*  |
| 1176w | 1180w | c\*  |
| 1334w | 1330w | CH2 bending | d\*  |
| 1449m | 1447m |
| - | 1590w | C=O, C=C and/or adsorbed H2O molecules and –COONa | e\*  |
| 1656s | 1657s |
| - | 2069m | Overtone and combination bands |
| 2376w | 2382w |
| 2516w | - | Aliphatic CH | f\*  |
| 2859w | - |
| 2926m | 2931s |
| 3422b | 3410b | Stretching vibration of OH and/or NH2 free or bonded | g\*  |
| w=weak, b=broad, s=strong, m=medium |

a\*: (Abd El-Mageed, Abd El-Salam, Abdel- Latif, & Mustafa, 2018)

b\*: (Monteiro & Neves, 2014)

c\*: (Paiva, 2007)

d\*: (Silverstein, Bassler, & Morill, 1974)

e\*: (Reddy & Lee, 2007)

f\*: (Asabe & Bashar, 2016)

g\*: (Rojas & Carlos 2019)

**Table S2: TGA data of the fabricated samples (hydrogel and grafted hydrogel).**

|  |  |
| --- | --- |
| **TGA parameters for polymeric samples** | **Comments** |
| **Hydrogel** | **grafted hydrogel** |
| Midpiont 0C | Approx. Wt. loss % | Midpiont 0C | Approx. Wt. loss % |
| 73 | 4 | 95 | 2 | Moisture losing  |
| 140 | 12 | 116 | 8 | Bonded water loss |
| 233 | 21 | 220 | 13 |
| 335 | 38 | 367 | 17 | Series of fragmentation of the polymer backbone depend on the bond strength between atoms |
| 371 | 50 | - | - |
| 403 | 52 | - | - |
| 422 | 63 | 441 | 55 |
| 466 | 72 | 460 | 60 |
| 703 | 90 | 725 | 60 | Complete degradation with carbonic residue is about 10% for hydrogel but for graft the residue is about 40%. |
| - |  | 821 | 60 |
| - |  | 918 | 60 |
| - |  | 952 | 60 |

**Table S3: Thermodynamic parameters**

|  |  |
| --- | --- |
| G (kJ mol-1)∆ | Thermodynamic parameters |
| Removal of iron | Removal of ammonia |
| -6332.12 | -1076.26 | 283 | Temperature K |
| -3795.64 | -1051.82 | 293 |
| -2042.85 | -1021.42 | 303 |
| -280.085 | -912.508 | 313 |
| -62.687 | -55.005 | ∆H (kJ mol-1) |
| -244.9 | -203.219 | S (J mol-1 K -1)∆ |

**Table S4: Kinetic models parameters data.**

|  |  |  |
| --- | --- | --- |
| **Parameter value** | **Parameter** | **Model** |
| **Iron removal** | **Ammonia removal** |
| 0.0283 | 0.0554 | k1(min-1) | **Pseudo-first order** |
| 128 | 254.6 | qe (mg g-1) |
| 0.98 | 0.8988 | R2 |
| 7.71 | 0.023 | k2(min-1) | **Pseudo-second order** |
| 0.295 | 1.06 | qe(exp) (mg g-1) |
| 0.36 | 1.469 | qe(cal) (mg/g) |
| 0.9979 | 0.9788 | R2 |