Table S1. Surface composition of NMF and A-NMF determined by XPS

|  |  |  |  |
| --- | --- | --- | --- |
| **Element** | **Binding Energy (eV)** | **% mass** | |
| **NMF** | **A-NMF** |
| Si (2p) | 102.5 | 10.01 | 22.96 |
| C (1s) | 285 | 47.95 | 1.98 |
| K (2p) | 293.8 | 0 | 11.98 |
| Ca (2p) | 347.4 | 1.05 | 7.85 |
| O (1s) | 531.7 | 29.86 | 48.05 |
| Al (2s) | 119.2 | 3.95 | 5.02 |

*Table S2: Mass Balance Results*

|  |  |  |  |
| --- | --- | --- | --- |
| **Ce** | **Ca + 0.5K** | **Qe (Zn)** | **% error** |
| 0 | 0.25 | 0.25 | 0.00 |
| 0.02 | 0.48 | 0.48 | 0.00 |
| 0.03 | 0.72 | 0.72 | 0.00 |
| 0.07 | 0.92 | 0.93 | 1.00 |
| 0.09 | 1.15 | 1.16 | 1.00 |
| 0.2 | 1.3 | 1.3 | 0.00 |
| 0.28 | 1.46 | 1.47 | 1.00 |
| 0.42 | 1.58 | 1.58 | 0.00 |
| 0.57 | 1.7 | 1.68 | 2.00 |
| 0.77 | 1.81 | 1.78 | 3.00 |
| 0.89 | 1.86 | 1.86 | 0.00 |
| 1.08 | 1.90 | 1.92 | 2.00 |
| 1.29 | 1.94 | 1.96 | 2.00 |
| 1.52 | 1.96 | 1.98 | 2.00 |
| 2.02 | 1.98 | 1.98 | 0.00 |
| 2.51 | 1.99 | 1.99 | 0.00 |
| 3.01 | 2.00 | 1.99 | 1.00 |
| 3.5 | 2.00 | 2.00 | 0.00 |
| 4 | 2.02 | 2.00 | 2.00 |
| 4.49 | 2.03 | 2.01 | 2.00 |
| 4.99 | 2.04 | 2.01 | 3.00 |

*Table S3: Tabulated Isotherm Model Results for Zinc*

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Langmuir** | **Freundlich** | **Redlich–Peterson** | **LF** | **Temkin** | **Toth** | **DR** |
| **Zinc** | | | | | | | |
| **SSE** | 0.17 | 0.61 | 0.13 | 0.10 | 0.67 | 0.11 | 0.17 |
| **Para-**  **meters** | **KL=** 25.27  **aL** = 12.47 | **aF** =1.69  **bF**=0.17 | **Kr** =33.6 **ar =** 17.4 **b =** 0.95 | **KLF =**12.7  **nLF** = 0.75  **aLF** = 5.93 | **B =** 0.20  **AT**= 447E3 | **Qm** = 2.18  **Kt**  =  0.12  **N**   =  0.66 | **Qm** =1.97  **E =** 112 |

*Table S4: Desorption Isotherm Model Results for Calcium and Potassium Desorption*

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Langmuir** | | **Freundlich** | **Redlich–Peterson** | **LF** | | **Temkin** | | **Toth** | **DR** |
| **Calcium** | | | | | | | | | | |
| **SSE** | 0.11 | 0.23 | | 0.07 | 0.05 | | 0.36 | | 0.06 | 0.13 |
| **Parameters** | **KL** =13.2  **aL** = 9.41 | **aF** =1.14  **bF**=0.19 | | **Kr**= 21.8 **ar=** 16.8 **b=** 0.92 | **KLF**=5.76  **nLF** = 0.66  **aLF** = 3.66 | | **B =** 0.15  **AT**=300E1 | | **Qm**= 1.62  **Kt** = 0.16  **N** = 0.55 | **Qm-**1.35  **E-** 104.5 |
|  | **Langmuir** | **Freundlich** | | **Redlich–Peterson** | **LF** | | **Temkin** | | **Toth** | **DR** |
| **Potassium** | | | | | | | | | | | |
| **SSE** | 0.04 | 0.36 | | 0.04 | | 0.04 | | 0.29 | 0.04 | 0.04 | |
| **Parameters** | **KL** = 23.9  **aL** = 18.7 | **aF** =1.11  **bF**=0.14 | | **Kr=** 23.4 **ar=** 18.2 **br=** 1.00 | | **KLF =**26.7  **nLF** = 1.03  **aLF** = 21.0 | | **B =** 1.04  **AT**=21.0 | **Qm** = 1.27  **Kt** = 0.05  **N**= 1.04 | **Qm**=1.26  **E=** 126 | |

*Table S5: Adsorption capacities of zinc from different models (experimental, desorption model, calculated Temkin model, and proposed composite equation)*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Ce** | **Qe exp** | **Qd-Ca + Qd 0.5K**  **(Desorption model)** | **Qe calculated**  **(Temkin model)** | **Qe composite**  **equation (5)** |
| 0.00 | 0.25 | 0.25 | 0.00 | 0.00 |
| 0.02 | 0.48 | 0.48 | 0.52 | 0.51 |
| 0.03 | 0.72 | 0.72 | 0.65 | 0.65 |
| 0.07 | 0.93 | 0.92 | 0.97 | 0.98 |
| 0.09 | 1.16 | 1.15 | 1.07 | 1.08 |
| 0.20 | 1.30 | 1.30 | 1.38 | 1.39 |
| 0.28 | 1.47 | 1.46 | 1.50 | 1.50 |
| 0.42 | 1.58 | 1.58 | 1.63 | 1.63 |
| 0.57 | 1.68 | 1.70 | 1.71 | 1.71 |
| 0.77 | 1.78 | 1.81 | 1.79 | 1.79 |
| 0.89 | 1.86 | 1.86 | 1.82 | 1.82 |
| 1.08 | 1.92 | 1.90 | 1.86 | 1.86 |
| 1.29 | 1.96 | 1.94 | 1.89 | 1.89 |
| 1.52 | 1.98 | 1.96 | 1.92 | 1.92 |
| 2.02 | 1.98 | 1.98 | 1.96 | 1.96 |
| 2.51 | 1.99 | 2.00 | 1.98 | 1.99 |
| 3.01 | 1.99 | 2.01 | 2.00 | 2.02 |
| 3.50 | 2.00 | 2.01 | 2.02 | 2.03 |
| 4.00 | 2.00 | 2.03 | 2.03 | 2.05 |
| 4.49 | 2.01 | 2.04 | 2.04 | 2.06 |
| 4.99 | 2.01 | 2.04 | 2.05 | 2.07 |
| **Mean Squared Error** | | 0.00 | 0.00 | 0.00 |

*Table S6: Optimization of adsorbent mass for a two-stage reactor for 99% zinc removal rate*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **C0 (mmol/L)**  (Initial conc) | **Single-stage**  **(experimental)** | **Two-stage reactor**  **(design)** | | | | |
| **m (g)**  (single stage) | **C1 (mmol/L)**  (Intermediate conc) | **C2 (mmol/L)**  (Final conc) | **M1 (g)**  (First stage) | **M2 (g)**  (Second stage) | **M1+M2 (g)**  (Total mass) |
| 0.25 | 0.176 | 0.016 | 0.003 | 0.017 | 0.009 | 0.026 |
| 0.5 | 0.118 | 0.032 | 0.005 | 0.025 | 0.006 | 0.031 |
| 0.75 | 0.104 | 0.048 | 0.008 | 0.035 | 0.006 | 0.041 |
| 1 | 0.101 | 0.063 | 0.010 | 0.046 | 0.005 | 0.051 |
| 1.25 | 0.104 | 0.079 | 0.013 | 0.056 | 0.006 | 0.062 |
| 1.5 | 0.109 | 0.095 | 0.015 | 0.067 | 0.006 | 0.073 |
| 1.75 | 0.116 | 0.111 | 0.018 | 0.078 | 0.006 | 0.084 |
| 2 | 0.124 | 0.127 | 0.020 | 0.088 | 0.007 | 0.095 |
| 2.25 | 0.133 | 0.143 | 0.023 | 0.099 | 0.007 | 0.106 |
| 2.5 | 0.142 | 0.158 | 0.025 | 0.110 | 0.008 | 0.118 |
| 2.75 | 0.152 | 0.174 | 0.028 | 0.121 | 0.008 | 0.129 |
| 3 | 0.162 | 0.190 | 0.030 | 0.132 | 0.009 | 0.141 |
| 3.25 | 0.172 | 0.206 | 0.033 | 0.143 | 0.009 | 0.152 |
| 3.5 | 0.183 | 0.222 | 0.035 | 0.154 | 0.010 | 0.163 |
| 4 | 0.204 | 0.254 | 0.040 | 0.175 | 0.011 | 0.186 |
| 4.5 | 0.225 | 0.285 | 0.045 | 0.197 | 0.012 | 0.209 |
| 5 | 0.247 | 0.317 | 0.050 | 0.219 | 0.013 | 0.232 |
| 5.5 | 0.269 | 0.349 | 0.055 | 0.241 | 0.014 | 0.255 |
| 6 | 0.292 | 0.380 | 0.060 | 0.263 | 0.016 | 0.278 |
| 6.5 | 0.314 | 0.412 | 0.065 | 0.284 | 0.017 | 0.301 |
| 7 | 0.336 | 0.444 | 0.070 | 0.306 | 0.018 | 0.324 |

*Table S7: Optimization of adsorbent mass for a two-stage reactor for different zinc removal rates.*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Concentration (mmol/L)** | **Two-stage adsorbent mass (g)** | | | | |
| **C0** | **99%** | **95%** | **90%** | **85%** | **80%** |
| 0.25 | 0.026 | 0.046 | 0.059 | 0.066 | 0.071 |
| 0.5 | 0.031 | 0.042 | 0.049 | 0.053 | 0.055 |
| 0.75 | 0.041 | 0.048 | 0.052 | 0.054 | 0.054 |
| 1 | 0.051 | 0.056 | 0.058 | 0.059 | 0.058 |
| 1.25 | 0.062 | 0.065 | 0.066 | 0.065 | 0.064 |
| 1.5 | 0.073 | 0.075 | 0.075 | 0.073 | 0.071 |
| 1.75 | 0.084 | 0.085 | 0.084 | 0.082 | 0.079 |
| 2 | 0.095 | 0.095 | 0.093 | 0.090 | 0.087 |
| 2.25 | 0.106 | 0.106 | 0.103 | 0.099 | 0.095 |
| 2.5 | 0.118 | 0.116 | 0.113 | 0.108 | 0.103 |
| 2.75 | 0.129 | 0.127 | 0.123 | 0.117 | 0.112 |
| 3 | 0.141 | 0.138 | 0.133 | 0.127 | 0.121 |
| 3.25 | 0.152 | 0.148 | 0.143 | 0.136 | 0.129 |
| 3.5 | 0.163 | 0.159 | 0.153 | 0.146 | 0.138 |
| 4 | 0.186 | 0.181 | 0.173 | 0.165 | 0.156 |
| 4.5 | 0.209 | 0.203 | 0.194 | 0.184 | 0.174 |
| 5 | 0.232 | 0.225 | 0.214 | 0.203 | 0.192 |
| 5.5 | 0.255 | 0.247 | 0.235 | 0.223 | 0.211 |
| 6 | 0.278 | 0.268 | 0.256 | 0.242 | 0.229 |
| 6.5 | 0.301 | 0.290 | 0.276 | 0.262 | 0.247 |
| 7 | 0.324 | 0.312 | 0.297 | 0.281 | 0.266 |

Chart

Description automatically generated Chart

Description automatically generated

Chart

Description automatically generated*Figure S1: Calcium desorption Isotherm modelling (a)- Langmuir, Freundlich, Redlich–Peterson–Peterson (b)-SIPS, Temkin, Toth, DR*

Chart

Description automatically generated

*Figure S2: Potassium desorption Isotherm modelling (a)- Langmuir, Freundlich, Redlich–Peterson–Peterson (b) SIPS, Temkin, Toth, DR*