**Supplementary material**

Phosphate removal performance and mechanism of Zirconium-doped magnetic gasification slag

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**Text S1: The adsorption capacity *q***

The adsorption amount *q*(mg/g) is computed according to the following equation (Abdellaoui et al., 2021):

(1)

where *Co, Ct* are respective phosphate concentrations (mg/L) of the initial and time *t* (h), *m*, *V* are the mass of sorbent (g) and the solution volume (mL), respectively. *q* (mg/g) indicates the amount of phosphate adsorbed per unit weight of adsorbent.

**Text S2: Phosphate species at different pH solution**

H3PO4, H2PO4-, HPO42- and PO43- are the main forms of the phosphate at different pH solution, which can be illustrated as follows (Abdellaoui et al., 2021; Xiong et al., 2017):

H3PO4 H++ H2PO4-  H++ HPO42-  PO43- + H+ (2)

where dissociation constant *pKa1, pK a2 and pK a3* are 2.15, 7.20 and 12.33, respectively.

**Text S3: Langmuir, Freundlich and Temkin isotherm equations**

The Langmuir and Freundlich non-linear equations can be expressed as follows (Arni et al., 2023; Sewu et al., 2017):

Langmuir isotherm equation:

(3)

Freundlich isotherm equation:

(4)

Temkin isotherm equation:

　 (5)

　 (6)

Where *Ce* (mg/L)represents the phosphate concentration at the equilibrium stage of sorption, *qe* and *qm* represents the sorption amounts of phosphate at equilibrium and the theoretical maximum monolayer sorption capacity, respectively, *KL* refers to the Langmuir constant, and measures the sorbent affinity to the solute. *KF* is the adsorption coefficient, *KT* represents Temkin constant, b represents heat of adsorption (J/mol).

**Text S4: kinetic model**

The non-linear equations of the three commonkinetic models can be displayed below (Akram et al., 2017; Liang et al., 2018)：

The pseudo first order equation:

= (5)

The pseudo second order equation:

(6)

The intraparticle diffusion model:

(7)

where *qe* and *qt* represent the respective adsorbed amount of phosphate at equilibrium and any time t (min). *k1, k2*and *kid* are the rate constants of the Eq. (5), Eq. (6) and Eq. (7), respectively. *C* represents the thickness of the boundary layer.



Fig.S1. The preparation process of samples.

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**Fig. S2.** The magnetic properties of co-precipitation of Zr and Fe (a) are stronger than loading Zr onto magnetic CGCS (after Fe) (b)

**Table S1**

Adsorption isotherm parameters. Adsorption conditions: reaction time, 24 h; sorbent dose, 1 g/L; initial phosphate concentration, 20-65 mg/L.

|  |  |  |
| --- | --- | --- |
| Isothermal model | Parameter | Value |
| Langmuir | *kL*(L/mg) | 0.384 |
| *qm*(mg/g) | 26.02 |
| R2 | 0.992 |
| Freundlich | *KF ((mg/g)/(mg/L)1/n)* | 14.07 |
| 1/n | 0.154 |
| R2 | 0.965 |
| Temkin | *KT*(L/mg) | 99.393 |
| A | 2.981 |
| R2 | 0.958 |

**Table S2**

Comparison of the adsorption capacity of GS-Z2M and adsorbents given in literatures for phosphate.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Adsorbent | Initial concentration  (mg P/L) | pH | Temperature  (°C) | Sorption capacity  (mg/g) | Ref. |
| Zr/Al-Mt | 20–50 | 5.0 | 25 | 17.2 | (Huang et al., 2015) |
| BFSs | 50-500 | 7.0 | 20 | 18.9 | (Kostura et al., 2005) |
| La-Ves | 1.02-5.03 | 7.1 | 25 | 6.7 | (Li et al., 2009) |
| Magnetic Fe–Zr binary oxide | 0-100 | 4.0 | 25 | 13.65 | (Long et al., 2011) |
| Iron oxide tailings | 5-150 | 6.6-6.8 | 20-21 | 8.2 | (Zeng et al., 2004) |
| Zr-CNTs | 5-50 | 3 | 30 | 10.9 | (Gu et al., 2019) |
| Lepidocrocite | 2–100 | 7.2 | 25 | 3.2 | (Sleiman et al., 2016) |
| ACF-LaFe | 5-60 | / | 25 | 29.44 | (Liu et al., 2013) |
| ACF-LaOH | 10-70 | / | 25 | 15.3 | (Zhang et al., 2012) |
| La-Z | 5-60 | 6.0 | 40 | 17.2 | (He et al., 2017) |
| La-FACC | 10-200 | / | 25 | 24.9 | (Asaoka et al., 2021) |
| MKC | 0-160 | 7.5 | 25 | 11.92 | (Deng and Shi, 2015) |
| GS-Z2M | 20-65 | 6 | 25 | 26.02 | This study |

**Table S3**

Adsorption kinetic parameters of GS-Z2M to phosphate.

|  |  |  |  |
| --- | --- | --- | --- |
| Kinetic models and Experimental results | Plot parameters | | Values |
| Experimental adsorption capacity | qe,exp (mg/g) | | 9.985 |
| Pseudo-first-order | *qe,cal*(mg/g) | | 9.889 |
|  | *K1*(min-1) | | 9.496 |
|  | *R2* | | 0.786 |
| Pseudo-second-order | *qe,cal*(mg/g) | | 10.021 |
|  | *K2*(min-1) | | 3.547 |
|  | *R2* | | 0.993 |
| Intraparticle diffusion | *Kid1*(mg/g min1/2) | | 1.403 |
|  | *C* | | 8.372 |
|  | *R2* | 0.977 | |
|  | *Kid2* (mg/g min1/2) | 0.107 | |
|  | *C* | 9.742 | |
|  | *R2* | 0.999 | |
|  | *Kid3*(mg/g min1/2) | 0.005 | |
|  | *C* | 9.968 | |
|  | *R2* | 0.999 | |

**Table S4**

Comparison of the toxic leaching results of GS-Z2M with the concentration limit of Class I surface water in China's surface water environmental quality standards. Units: mg/L.

|  |  |  |
| --- | --- | --- |
| Element | Concentration leached from GS-Z2M | Concentration limit for Class I surface water |
| As | < 0.0004 | 0.05 |
| Hg | < 0.00002 | 0.00005 |
| Cr | 0.0043 | 0.01 |
| Ni | 0.00096 | 0.02 |
| Cu | < 0.00053 | 0.01 |
| Zn | < 0.00031 | 0.05 |
| Cd | < 0.00006 | 0.01 |
| Pb | < 0.00008 | 0.001 |

**Table S5**

Comparison of leaching results of iron and zirconium from GS-Z2M.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Element | Water type | Units | Concentration at pH 3 | Concentration at pH 3 |
| Fe | DI water | mg/L | 1.02 | < 0.03 |
| Zr | Phosphate solution | μg/L | 0.14 | < 0.02 |

**Table S6** Main components of actual wastewater.

|  |  |  |
| --- | --- | --- |
| Main components | Units | Content |
| Ca2+ | mg/L | 60.3 |
| K+ | mg/L | 10.1 |
| Mg2+ | mg/L | 24.5 |
| Na+ | mg/L | 74.7 |
| NH4+ | mg/L | 5.4 |
| Cl- | mg/L | 120.3 |
| NO3- | mg/L | 10.6 |
| SO42- | mg/L | 80.2 |
| DOC | mg/L | 6.3 |
| PO43- | mg/L | 1.5 |
| pH | / | 7.4 |

**Table S7**

BET specific surface area and BJH pore parameters of CGCS and GS-Z2M.

|  |  |  |  |
| --- | --- | --- | --- |
| Sample | BET specific surface area (m2/g) | BJH average pore diameter (nm） | BJH cumulative volume of pores (cm3/g) |
| CGCS | 10 | 6.73 | 0.0129 |
| GS-Z2M | 188 | 5.22 | 0.2097 |

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