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Electronic Supplementary Information for

Al-substitution-induced defect sites enhance adsorption of Pb²⁺ on hematite

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Figure s1. Hematite structure with (001) facets on the side (a) and top view (b). The directions of the crystallographic axes are also shown for reference.



Figure s2. (a-c) Nitrogen adsorption-desorption isotherms of H-0, H-5 and H-10. Insets: Pore volume distribution curves.



Figure s3. Relative charge density (mC/m²) as a function of pH at 0.01 mol/L $\ensuremath{\text{KNO}_3}.$

| | | samples. | | |
|--------|--------|-----------------|------|---------|
| Sample | B.E/eV | Surface | FWHM | Percent |
| | | Species | eV | % |
| | 530.01 | O ²⁻ | 1.97 | 67.04 |
| | 531.01 | OH- | 1.97 | 22.32 |
| H-0 | 532.53 | H_2O | 2.22 | 10.64 |
| | 529.84 | O ²⁻ | 1.97 | 58.69 |
| | 531.03 | OH- | 1.97 | 22.53 |
| H-5 | 532.54 | H_2O | 2.22 | 17.87 |
| | 529.86 | O ²⁻ | 1.97 | 37.01 |
| | 531.08 | OH- | 1.97 | 39.38 |
| H-10 | 532.79 | H_2O | 2.22 | 23.60 |

Table s1. Fitting parameters used for O (1s) spectra of Al-doped hematite

Table s2. Langmuir fitting parameters for Pb²⁺ adsorption onto Al-substituted

| hematite | | | | | | | | |
|----------|-----|-------------------------|---------------|---------|-----------------------|--|--|--|
| annalaa | nIJ | K(L/mg ²) - | Qmax | | D ² | | | |
| samples | рп | | $\mu mol/m^2$ | mmol/kg | K- | | | |
| Н-0 | 5 | 13.64 | 0.82 | 22.76 | 0.90 | | | |
| | 6 | 12.64 | 6.49 | 158.64 | 0.95 | | | |
| H-5 | 5 | 8.06 | 1.23 | 32.51 | 0.96 | | | |
| | 6 | 23.6 | 6.98 | 184.31 | 0.96 | | | |
| H-10 | 5 | 7.21 | 3.51 | 109.70 | 0.96 | | | |
| | 6 | 13.8 | 10.46 | 289.45 | 0.97 | | | |