



## Supplementary Materials

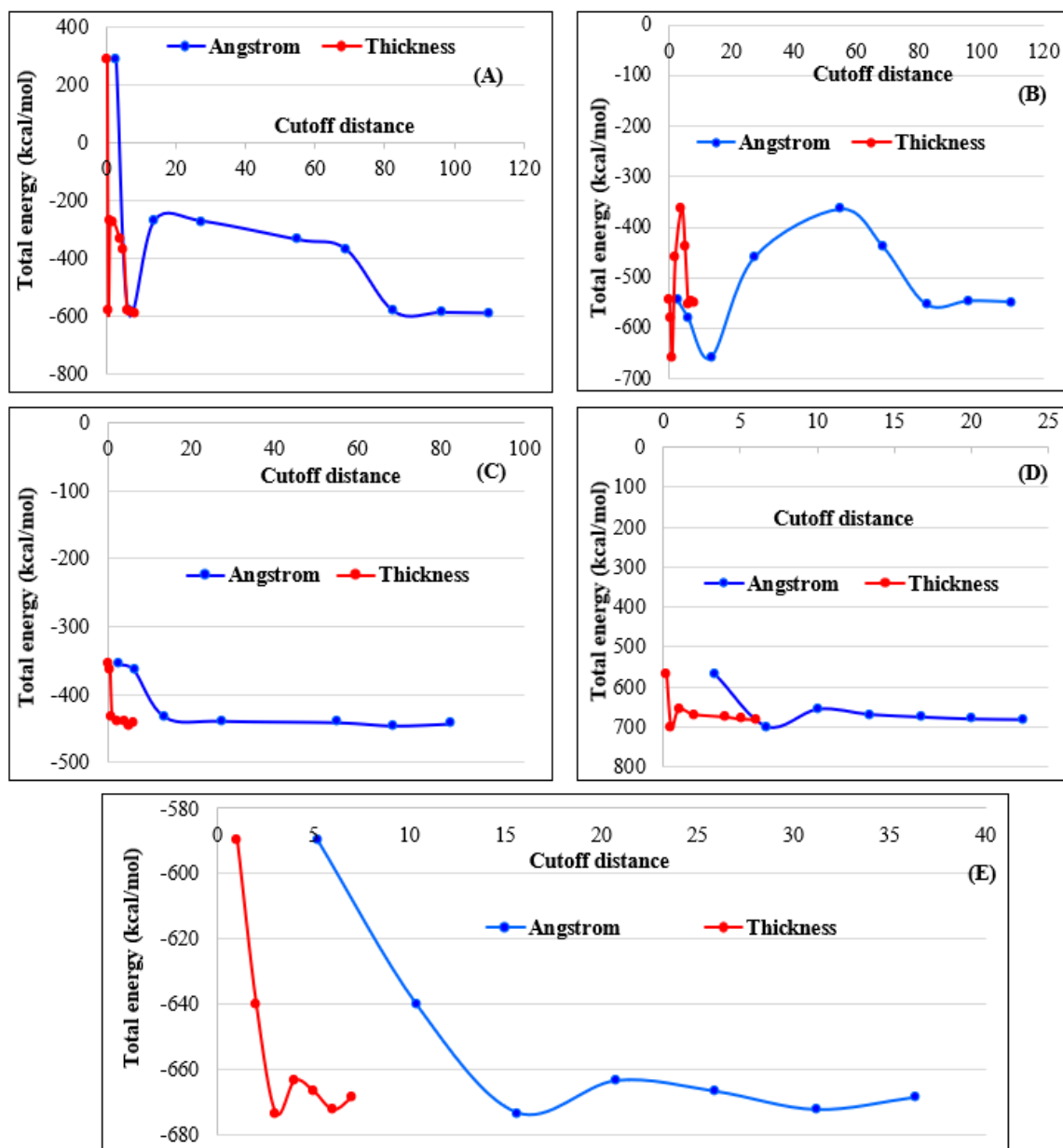
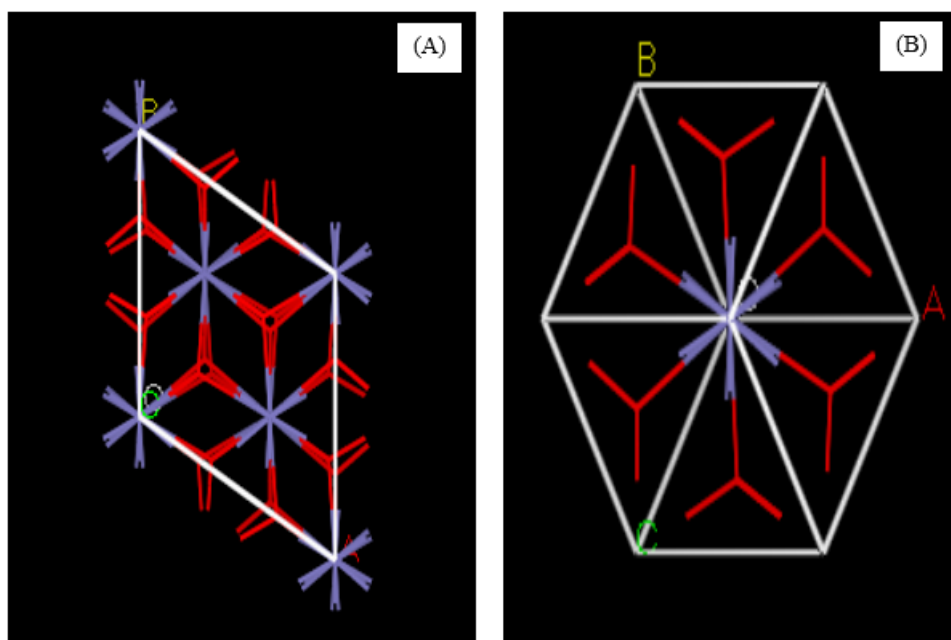
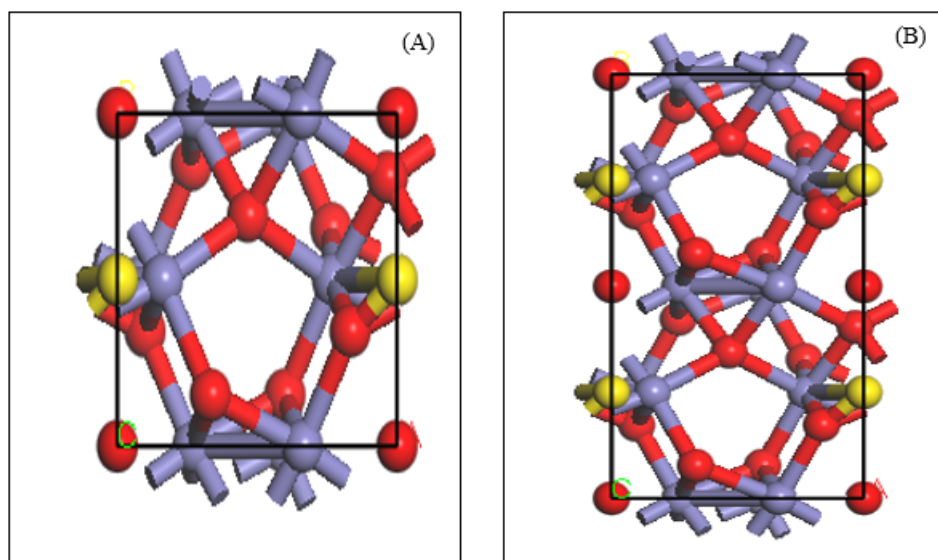


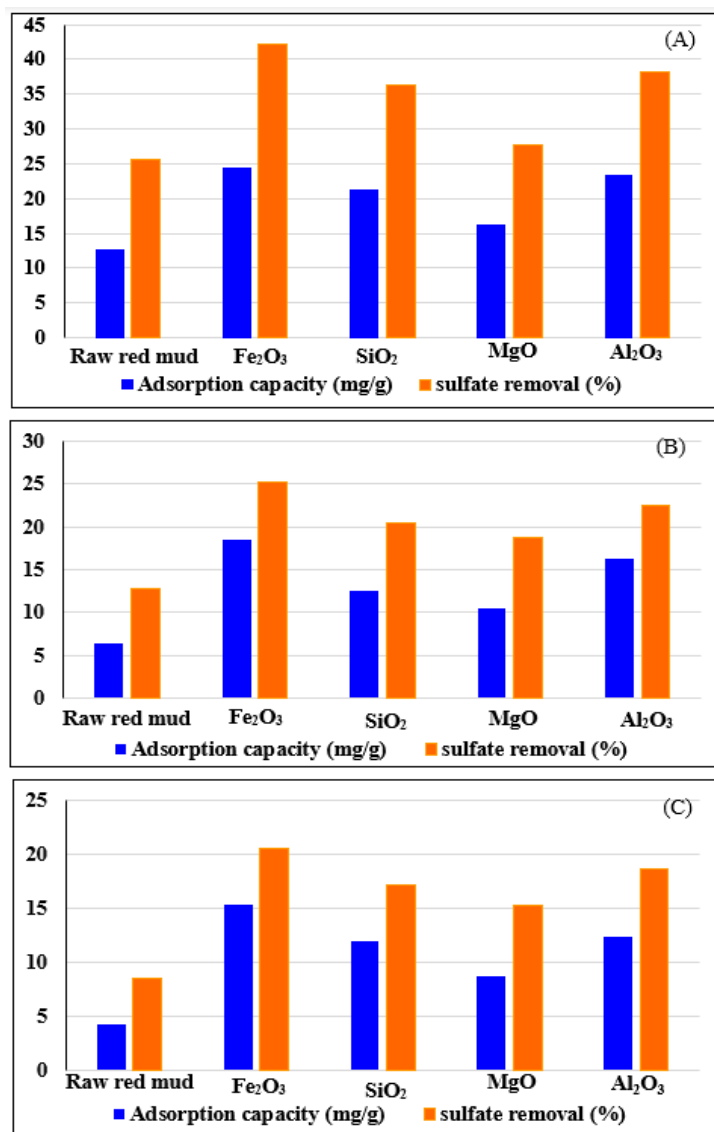
Fig. S1. Adsorption energy per unit of sulfate ion for Fe<sub>2</sub>O<sub>3</sub> (A), Al<sub>2</sub>O<sub>3</sub> (B), CaCO<sub>3</sub> (C), SiO<sub>2</sub> (D), and TiO<sub>2</sub> (E).



**Fig. S2.** Optimized rhombohedral (A) and hexagonal (B) crystal network modeling.



**Fig. S3.** Addition of sulfate ions to 1x1 hematite surface (A) and the 2x1 hematite surface (B).



**Fig. S4.** Adsorption capacity and sulfate removal percentage for different metal oxides and red mud at pH 5 (A), pH 6 (B), and pH 7 (C).

**Table S1.** Effect of pH on sulfate removal and sorption capacity by RM (adsorbent 2 g/L, contact time of 60 min, sulfate concentration of 1000 ppm and temperature 27°C).

pH	4	5	6	7	8	9	10
Sulfate removal (%)	18.92	31.98	20.01	17.84	15.66	2.61	1.56
Capacity adsorption (mg/g)	9.46	15.99	10	8.9	7.83	1.3	1.1

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**Table S2.** Effect of the Sulfate concentration on sulfate removal and sorption capacity by RM (adsorbent 2 g/L, contact time of 60 min and temperature of 27 °C).

Sulfate concentration (ppm)	100	250	500	750	1000	1500	2000
Sulfate removal (%)	1.15	3.99	13.45	20.54	26.47	23.15	26.83
Capacity adsorption (mg/g)	1.15	3.52	12.5	21.71	29.35	25.24	29.65

**Table S3.** Effect of adsorbent dosage on sulfate removal and sorption capacity by RM (contact time of 15 min, sulfate concentration of 1000 ppm and temperature of 27 °C).

Adsorbent dosage (g/L)	0.5	1	2	3	4	5
Sulfate removal (%)	1.22	1.46	3.45	5.16	6.32	6.5
Capacity adsorption (mg/g)	1.1	1.45	3.16	1.03	1.9	2.1

**Table S4.** Effect of the contact time on sulfate removal and sorption capacity by RM (adsorbent 2 g/L, sulfate concentration of 1000 ppm and temperature of 27 °C).

Contact time (min)	10	20	30	45	60	120
Sulfate removal (%)	1.98	6.12	8.19	10.3	12.2	24.71
Capacity adsorption (mg/g)	3	4.15	11.04	7.55	6.45	5.23