Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Supplementary Information:

Atmospheric fates of SO_2 at the gas-solid interface of iron oxyhydroxide (FeOOH) minerals: effects of crystal structure, oxalate coating and light irradiance

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Table S1. Parameters for uptake coefficient calculation

Parameter (unit)	Value
Sulfate formation rate: $d[SO_4^{2-}]/dt$ (ion s^{-1})	According to reactions
A_{BET} (m^2 g^{-1})	Shown in Table 1
A_{geo} (m^2)	1.96×10^{-5}
Reactant concentration: C_{SO_2} (molecule m^{-3})	1.96×10^{20}
Gas constant: R (J mol^{-1} K^{-1})	8.314
Temperature: T (K)	298
Molar mass: M_{SO_2} (Kg mol^{-1})	6.4×10^{-2}
π	3.14

Table S2. Assignment of vibrational frequencies of adsorbed surface sulfur-containing products upon exposure of SO_2 on Fe (oxyhydr)oxides nanoparticles.

Surface Species Description	Vibrational Mode	Assignment Frequency[a] (cm^{-1})	Refs
Sulfate	Symmetric stretching vibration modes of S=O	1270	1
Bidentate Sulfate	v_3 symmetric modes	1190, 1158, 1097	1-3
Bridging (bi)sulfate		1050, 1010	4
Chemisorbed (bi)sulfite	v_1 and v_3 modes of sulfite	971, 923, 886	5

[a]These frequencies of IR bands of sulfur-containing species refer to the frequencies of observed surface product in this work, which are close to the frequencies documented by early literature.

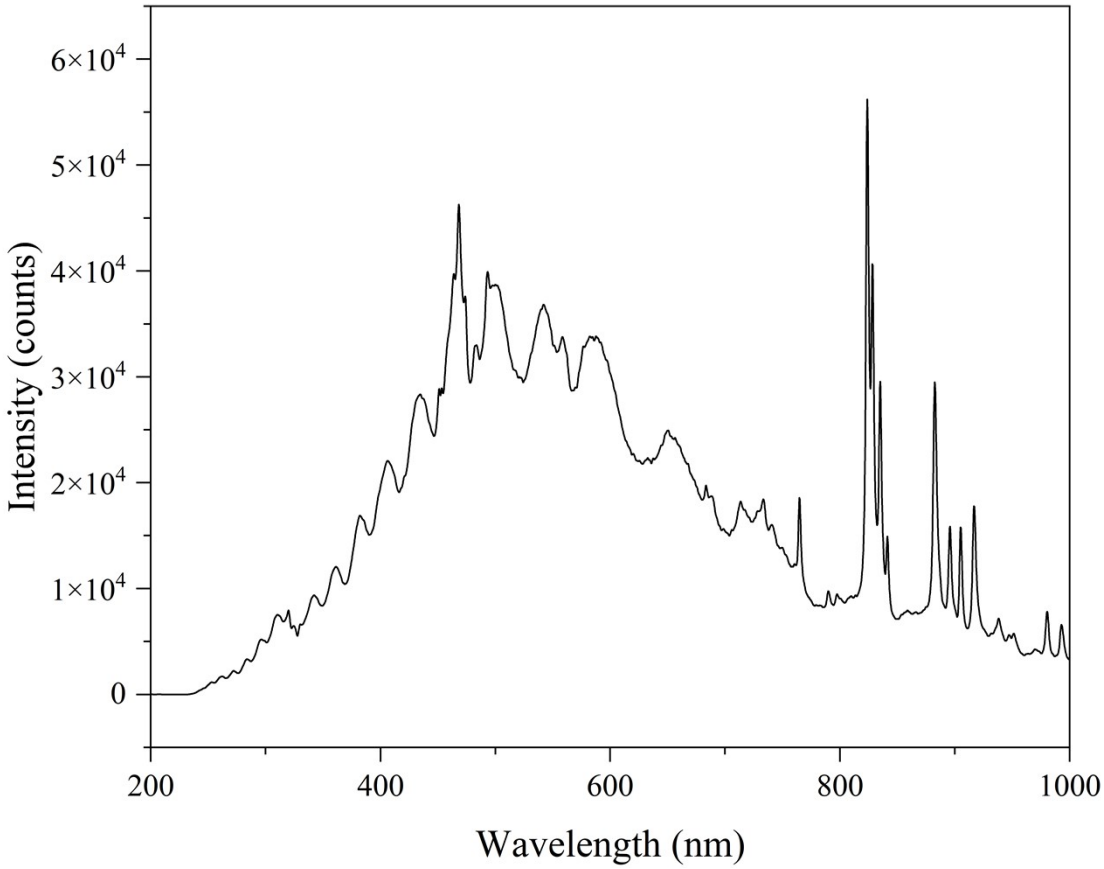

Fig. S1. The spectrum of the xenon lamp (TCX250).

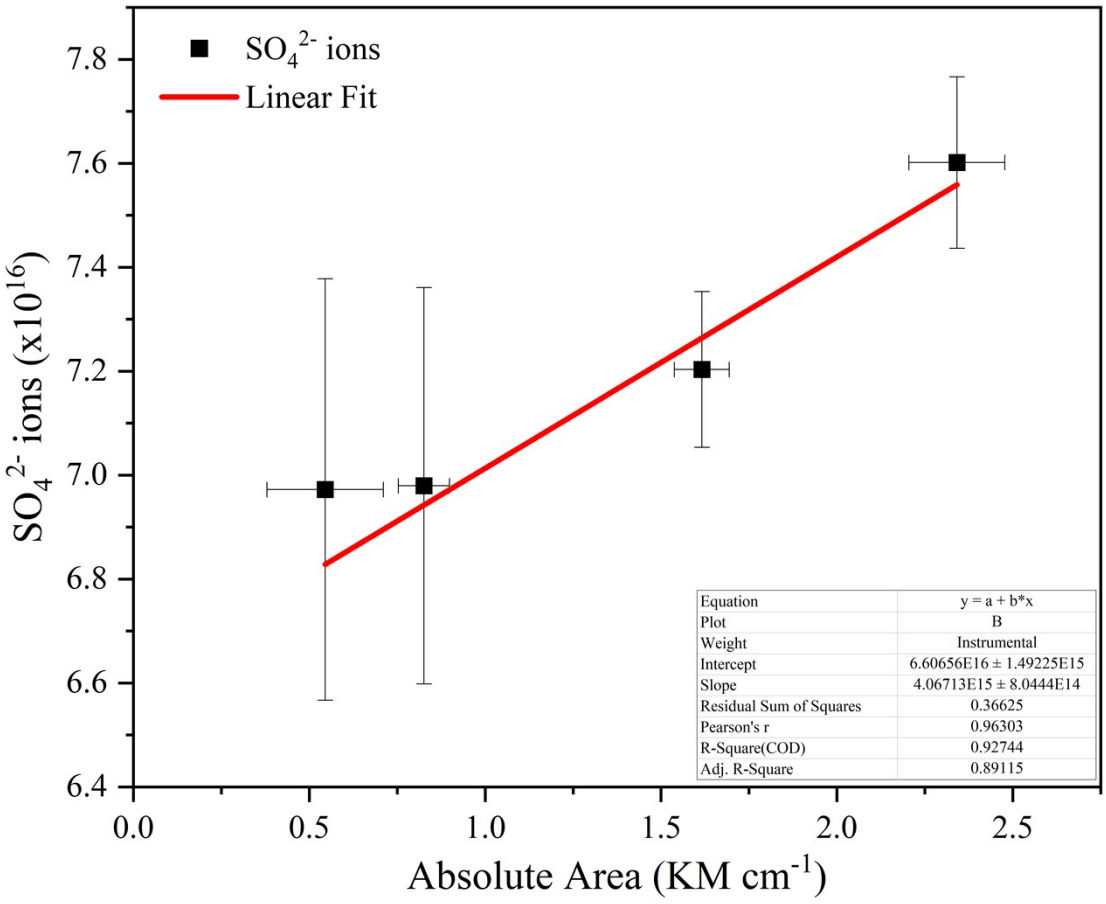

Fig. S2. Calibration plot for Conversion-factor of molecules of SO_4^{2-} used in α-FeOOH infrared experiments versus corresponding integrated area of KM.

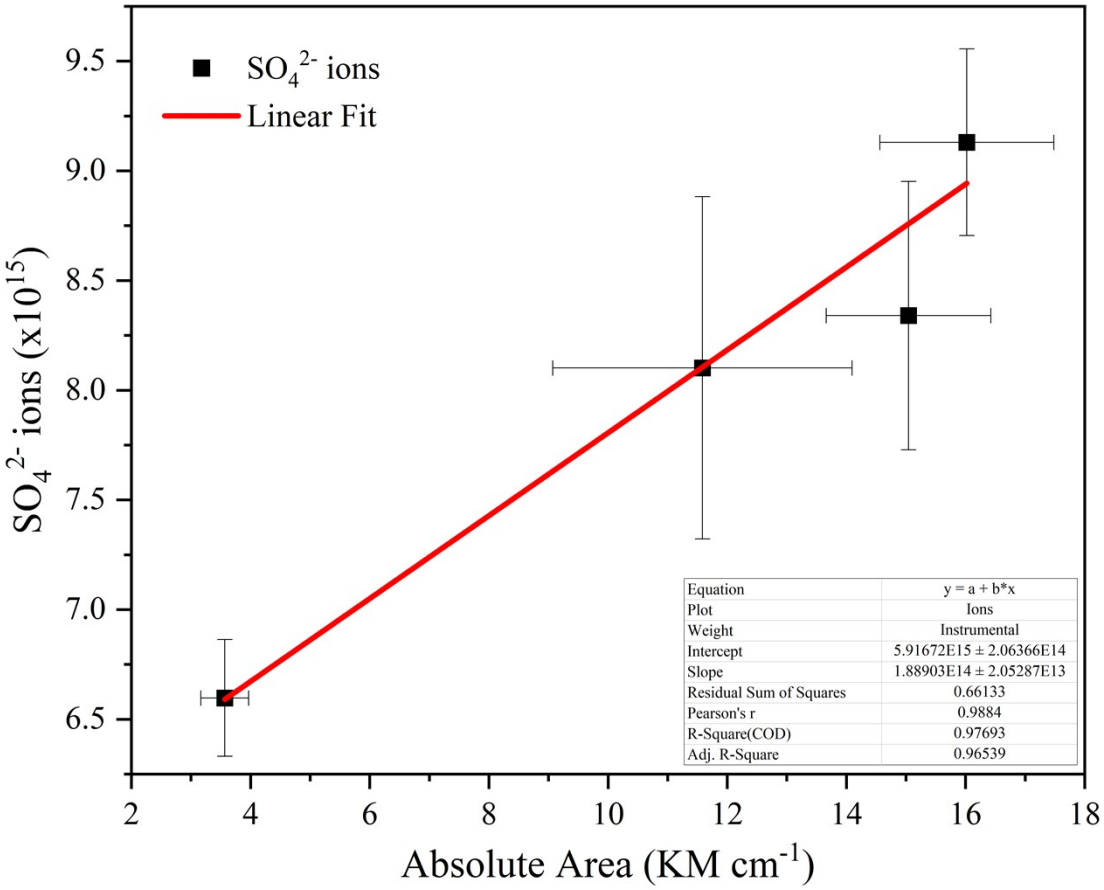

Fig. S3. Calibration plot for Conversion-factor of molecules of SO_4^{2-} used in β-FeOOH infrared experiments versus corresponding integrated area of KM.

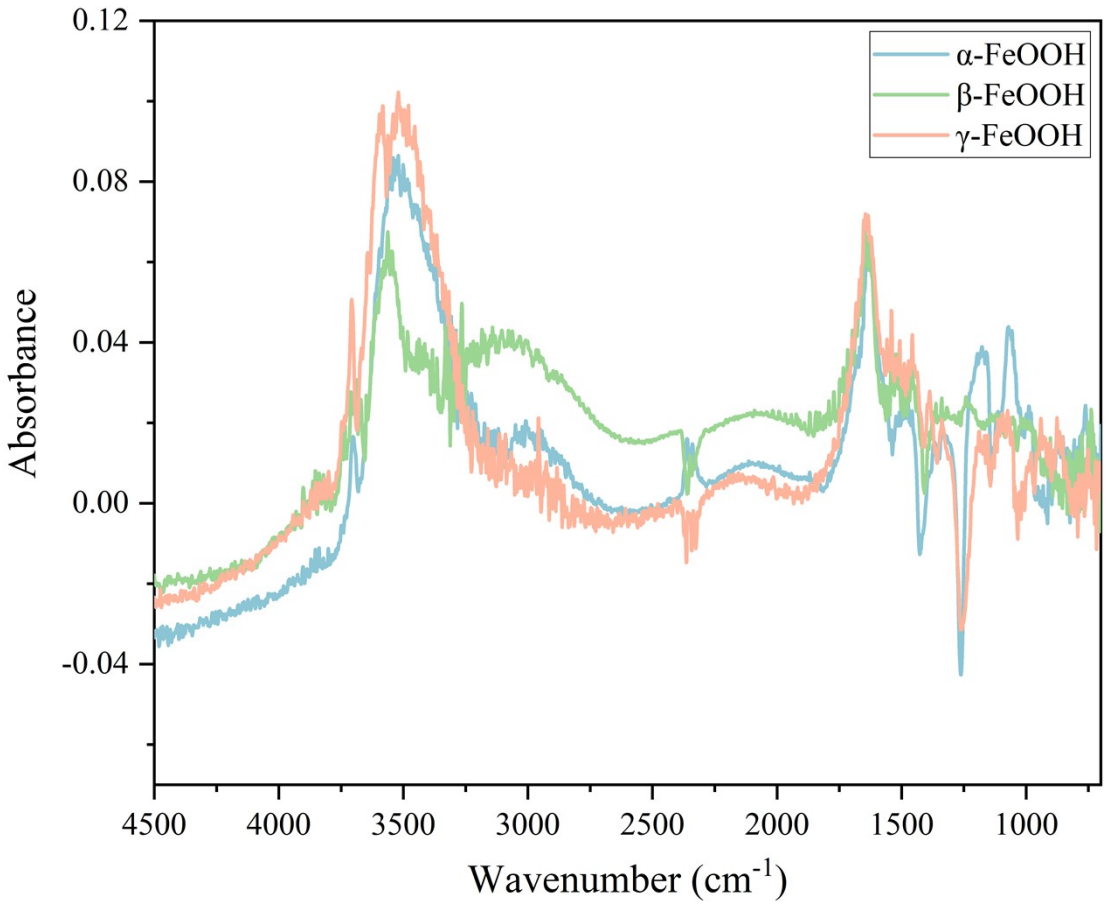

Fig. S4. Raw in situ DRIFTS spectra (4500-700 cm^{-1}) collected for the three pristine samples at 60 min under dark condition.

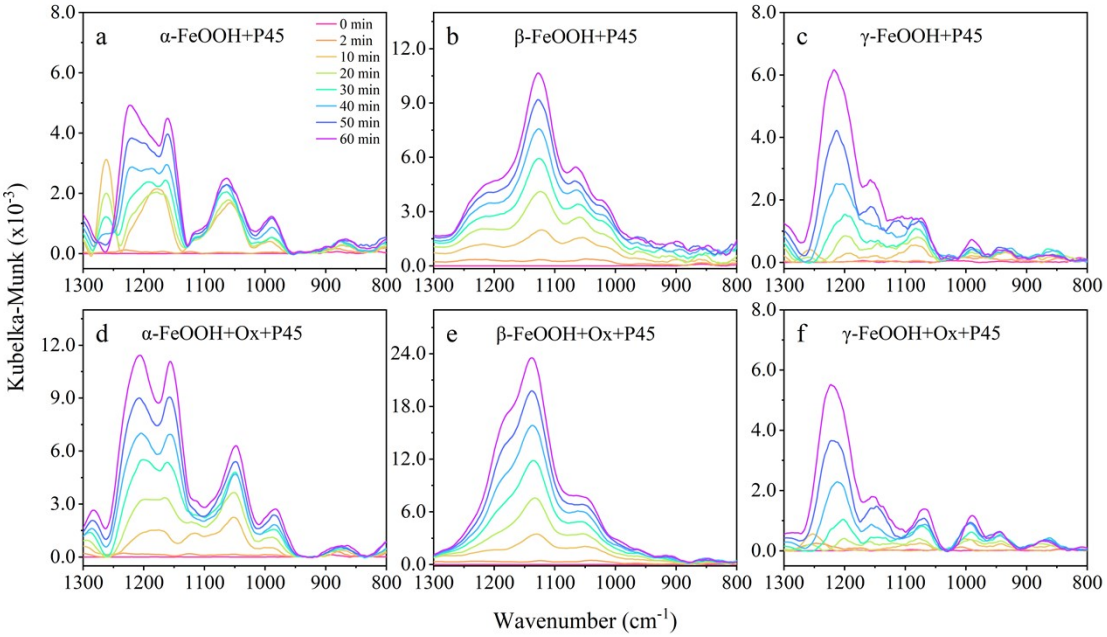

Fig. S5. In situ DRIFTS spectra collected for the three (a, b, c) pristine and (d, e, f) oxalate-coating samples under light irradiation (P45): (a, d), α-FeOOH. (b, e), β-FeOOH. (c, f), γ-FeOOH.

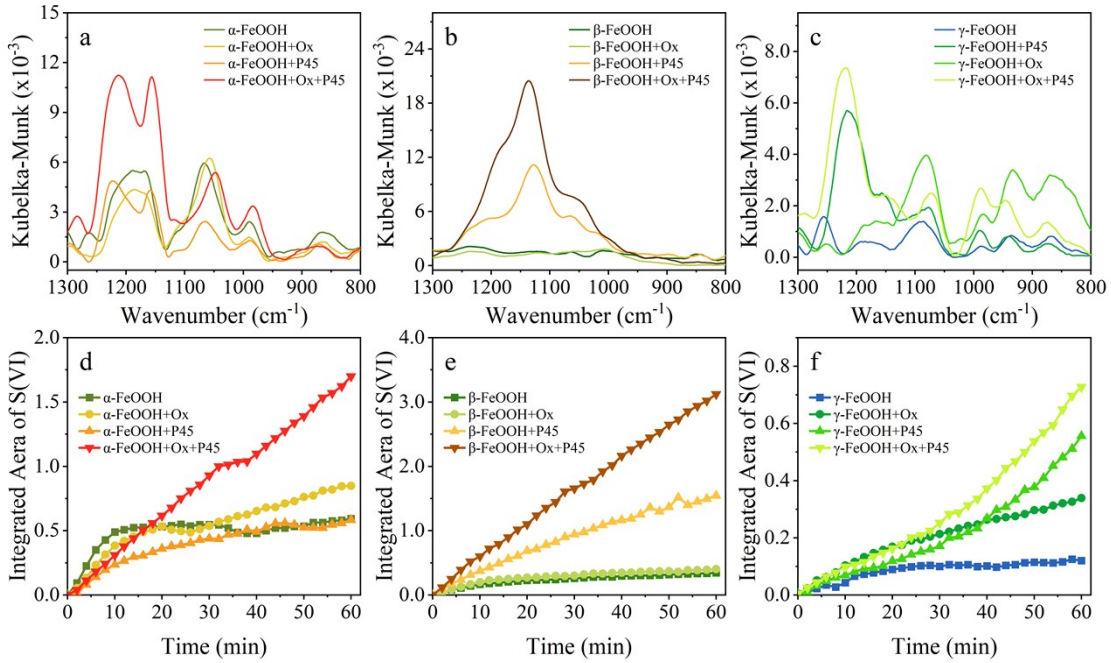

Fig. S6. In situ DRIFTS spectra of α-FeOOH (a), β-FeOOH (b) and γ-FeOOH (c) at 60 min under different conditions and the corresponding integrated areas of sulfate for α-FeOOH (d), β-FeOOH (e) and γ-FeOOH (f) within 60 min.

References

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