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Revealing Interfacial Interactions in PFOA Adsorption on Dolomite: A Molecular and Experimental Investigation for Advanced Water Treatment

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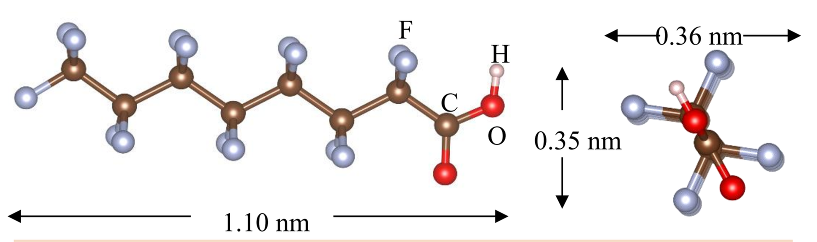
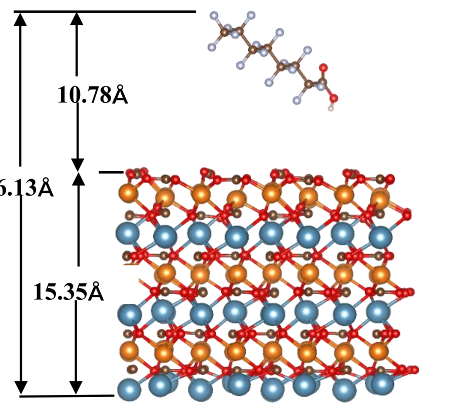
INTRODUCTION & AIM

PFOA is **persistence and widespread contamination** in water system. The methods studied at present are **expensive** or have **high technical requirements** (e.g., MOF, GAC, Biomaterials et al.)[1-3].





Dolomite is easy to obtain due to its abundant resources and low cost, and is '**GREEN**' and '**NATURE**' materials[4-6].

Significance:
This study **fills a research gap** in the field of natural minerals without modification for PFOA (see Figure S1), broadening the potential applications of our research in environmental remediation.

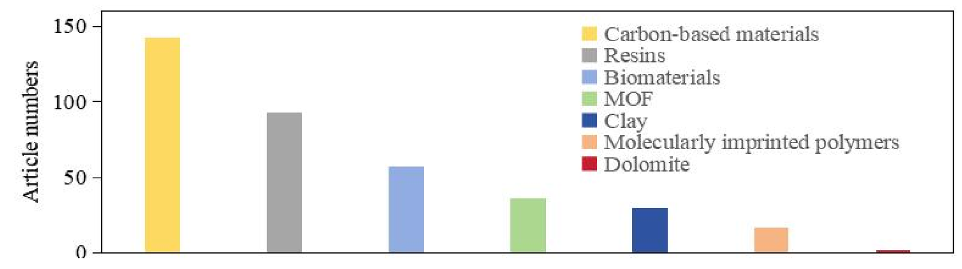
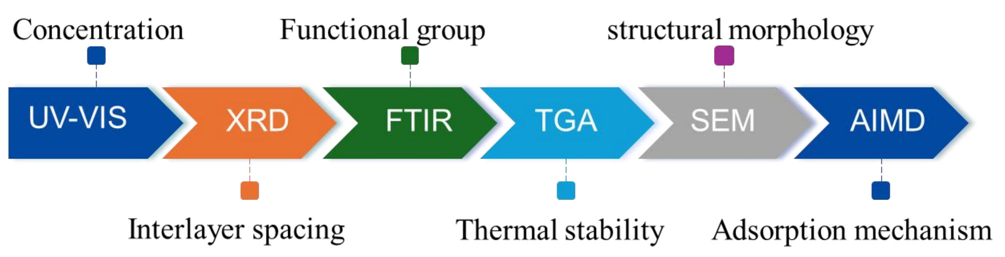


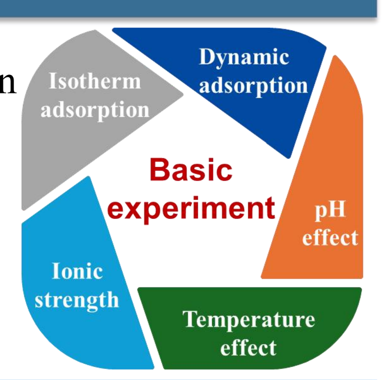
Figure. S1 Natural minerals without modification for PFOA

METHOD



the initial concentration of PFOA

- Isotherm adsorption: 0 ~ 200 mg L^{-1}
- other experiment: 100 mg L^{-1}



The experimental **solid-liquid ratio** was **20ml/g**.

RESULTS & DISCUSSION

3.1. Basic Experiment

- Variations in ionic strength had **negligible** impact on PFOA adsorption for DL and CDL (Fig. 1c).
- The adsorption capacity of PFOA increased with temperature (Fig. 1d), confirming an **endothermic process** (DL:ΔH=6.21 kJ mol^{-1}; CDL: ΔH=34.01 kJ mol^{-1}) (Fig. 1d).
- The adsorption capacity of PFOA on DL and Zate decreased with increasing pH (Fig. 1e, 2a). XRD confirmed that the structures of DL and CDL remained intact (Fig. 2a, b). Calcination shifted DL's surface charge from negative to positive (Fig. 1f), enabling **efficient capture of PFOA$^-$ via electrostatic attraction**.

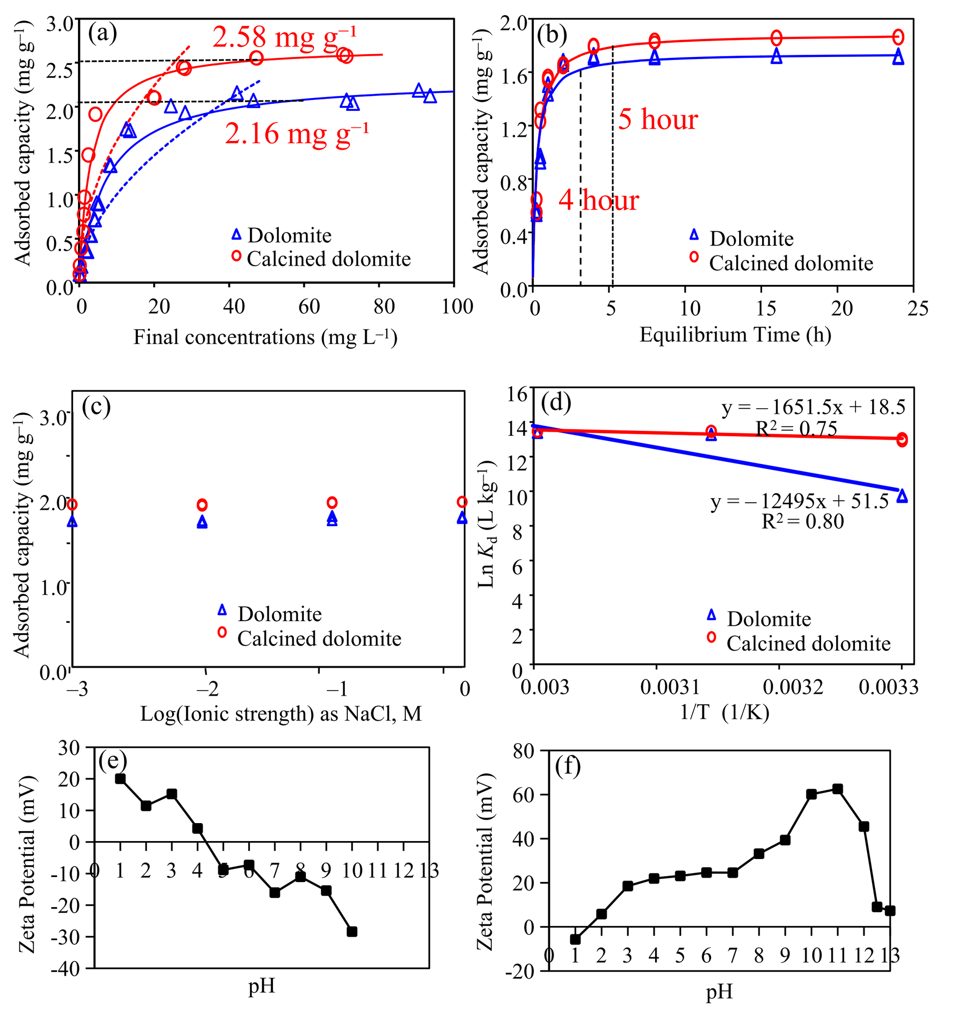


Fig. 1. Adsorption of PFOA on dolomite and calcined dolomite.

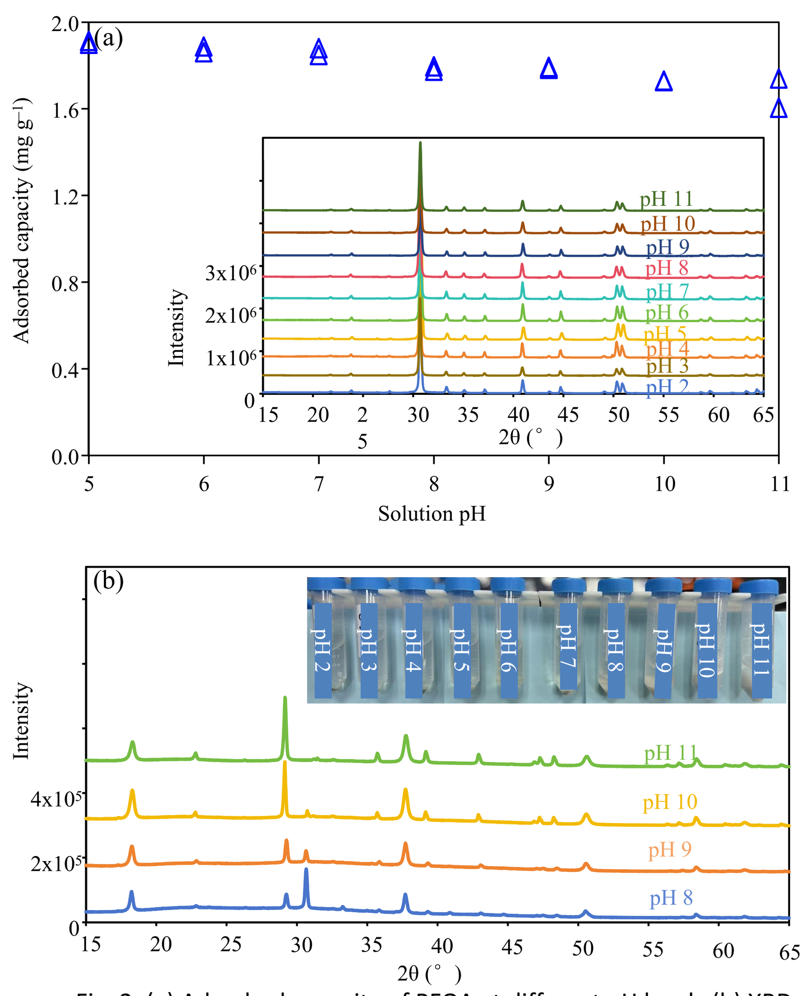


Fig. 2. (a) Adsorbed capacity of PFOA at different pH levels.(b) XRD patterns of dolomite samples treated.

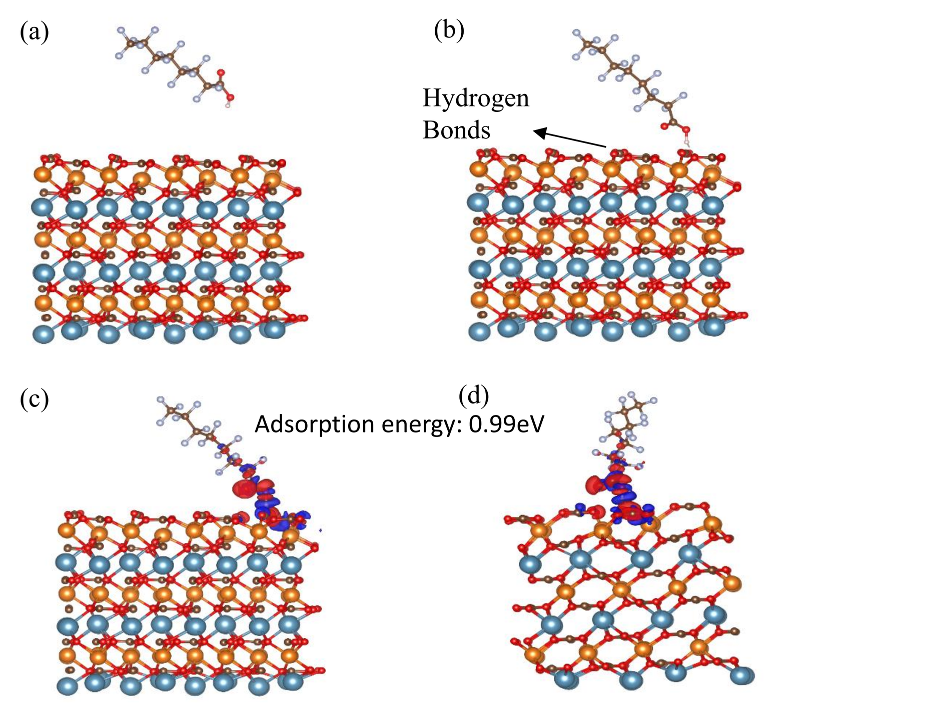


Fig. 3. The formation of hydrogen bonds between PFOA molecule and dolomite surface during an AIMD simulation (a and b). Polarization analysis showing charge accumulation (red) and depletion (blue) in PFOA and dolomite (c and d).

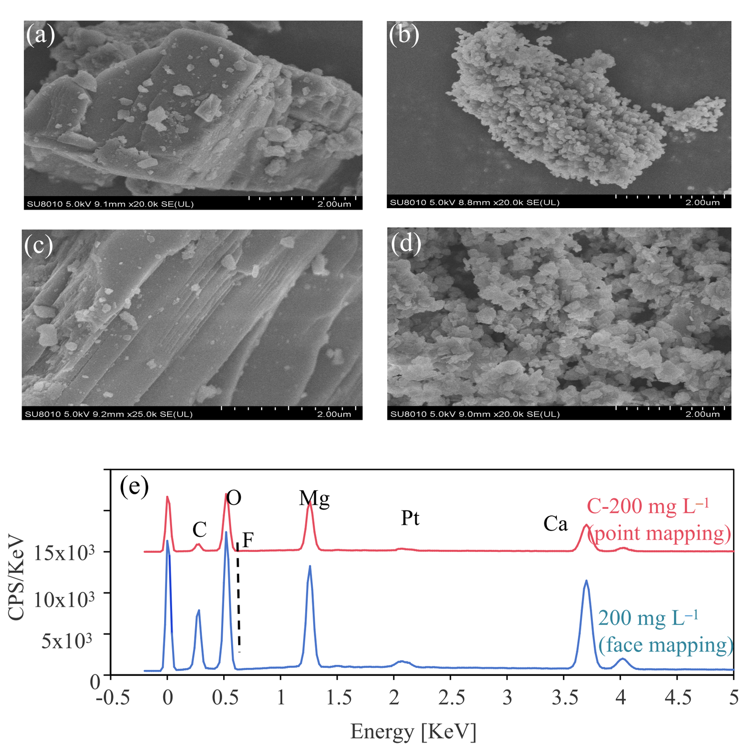


Fig. 4. SEM images of raw dolomite (a), raw calcined dolomite (b), and their adsorbed samples, respectively (c, d). The EDS spectra of face and point mapping of them (e). (C signal represents calcined)

3.2. Molecular simulation, SEM, EDM

The adsorption mechanism involves **hydrogen bonds**, **polarization** and **charge transfer** (Fig. 3).

The **structure of calcined dolomite changes** after adsorption by PFOA (Fig. 4).

3.3. FTIR, XRD, TGA, DTG

After calcination, dolomite is transformed into **calcium hydroxide** and **magnesium hydroxide** [7], increasing surface porosity and adsorption sites. And some of dolomite will partially transform into **calcite** [8] (Fig. 5).

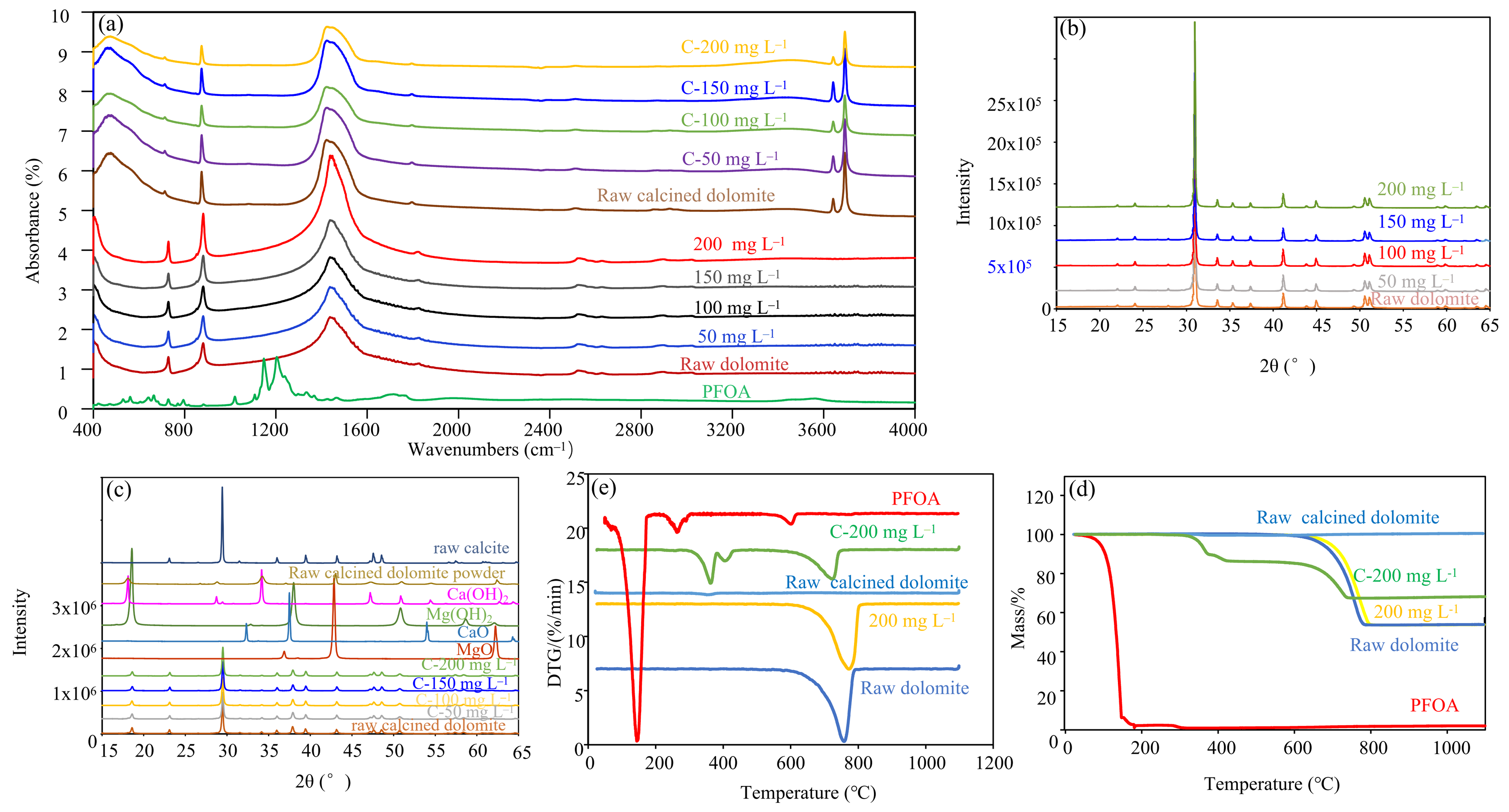
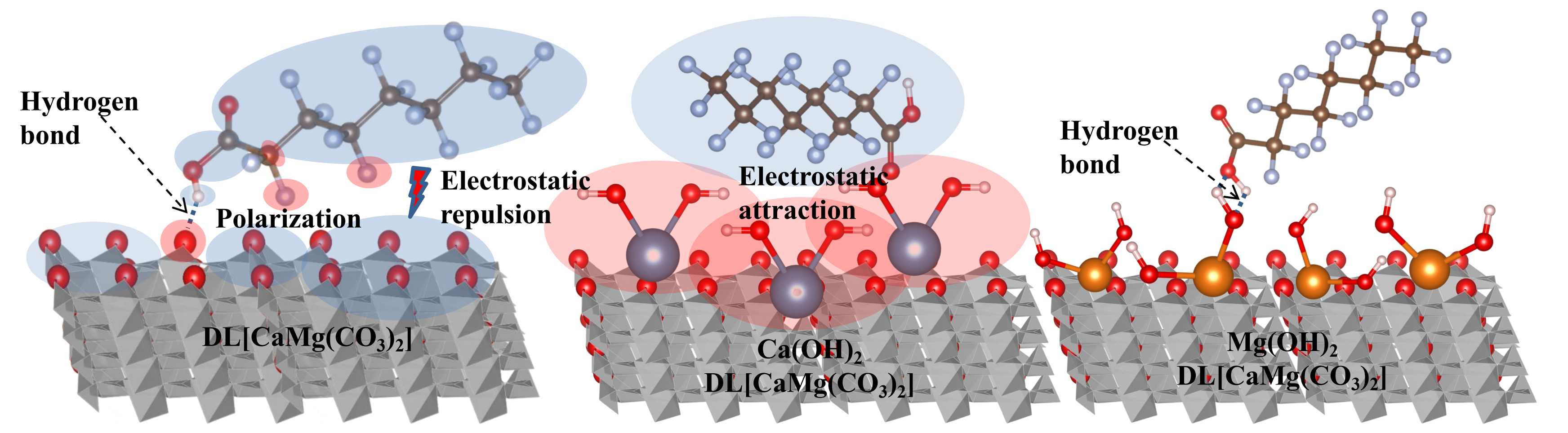
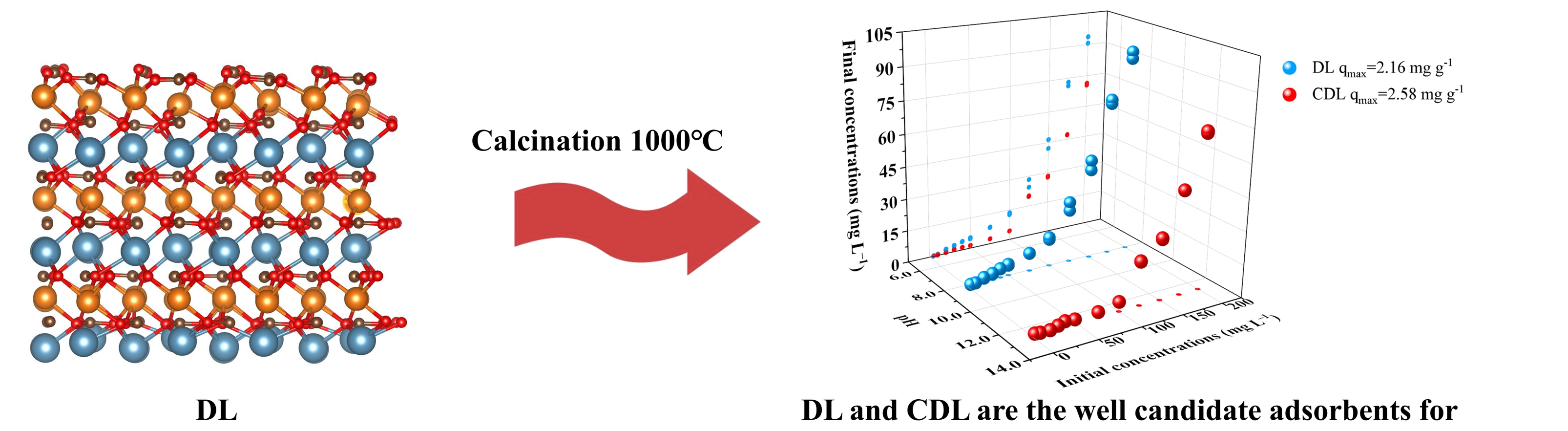


Fig. 5. (a) FTIR spectra of raw dolomite, raw calcined dolomite and adsorbed samples , respectively. The color numbers are the initial concentrations. XRD patterns of dolomite (b) and calcined dolomite (c) , respectively. TGA (d) and DTG (e) analyses of dolomite and calcined dolomite.

CONCLUSION

- **Molecular simulation for elucidation of the adsorption mechanism**: The main adsorption mechanism of perfluorooctanoic acid (PFOA) on dolomite and calcined dolomite is **electrostatic attraction** and **hydrogen bonding**.
- **Molecular-Level Analysis**: Through detailed characterization using advanced analytical techniques (SEM, TGA, XRD, and FTIR), we provide **novel perspectives on the molecular-level processes** involved in adsorption.
- **Bridging Science and Application**: By developing **low-cost**, **Green, natural, abundant reserves of dolomite** in nature and comprehensively evaluating their adsorption performance under various physicochemical conditions.
- **Performance Optimization**: Our **comprehensive evaluation** of adsorption performance under various conditions (kinetics, initial PFOA concentration, temperature, pH, and ionic influence) provides valuable data for optimizing the use of dolomite in diverse environmental scenarios.
- **Sustainable Solution**: The development of dolomite from readily available, environmentally friendly materials **offers a sustainable approach for addressing the critical issue of PFOA** contamination, thereby aligned with global efforts towards greener technologies in environmental remediation.





FUTURE WORK

In order to improve the adsorption rate of dolomite to PFOA, we may conduct composite microbeads (**dolomite/sodium alginate**) experiments in future work and apply them in **practical applications**.

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