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Invited review

Microscopic-scale modeling of CO_2 sequestration and enhanced oil recovery: Methods, mechanisms, and challenges

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Abstract:
Addressing climate change urgently requires innovative strategies for carbon capture, utilization, and storage (CCUS), with CO_2-enhanced oil recovery (EOR) serving a dual role in decarbonization and energy security. Optimizing these technologies hinges on decoding the microscopic mechanisms-adsorption, mineralization, wettability alteration, and multiphase transport-that govern macroscopic reservoir behavior. This review synthesizes advances in computational modeling tools-molecular dynamics (MD), density functional theory (DFT), deep learning (DL), and Monte Carlo (MC) methods-that unravel these complex physicochemical interactions. MD simulations can resolve nanoconfined fluid dynamics and interfacial phenomena under reservoir conditions, while DFT offers quantum-level insights into adsorption energetics and reaction pathways at mineral-fluid interfaces. DL models enable rapid property prediction, inverse material design, and surrogate modeling, and MC efficiently predicts thermodynamic equilibria in nanoporous media. Together, these methods bridge angstrom-scale chemistry to pore-scale phenomena, enabling predictive insights into CO_2 trapping, mineralization, and hydrocarbon displacement. Synergistic integrations of these approaches (such as DL-potentials for MD or DL-driven analysis of MC datasets) transcend individual limitations, enabling predictive, high-fidelity modeling from atomic bonding to pore-scale transport. Despite these synergies, key challenges remain. Bridging the temporal gap between femtosecond-scale simulations and field-scale, addressing data scarcity in geologically heterogeneous systems, and reconciling simulations with macroscopic experimental observations all require continued innovation. Emerging solutions include machine learning-based interatomic potentials, active and adaptive sampling, and exascale computing architectures capable of modeling billion-atom systems with mesoscale fidelity. The future of CO_2-EOR and geologic sequestration lies in tightly coupled, closed-loop frameworks that integrate molecular simulations, reactive transport models, and real-time field data. Platforms like the Illinois Basin Decatur Project provide essential benchmarks for validating models against in situ behaviors, while community-driven databases and federated learning enhance model generalizability and reproducibility. Ultimately, model-informed experimental design-guided by DL-predicted materials and MD-derived fluid behavior-will accelerate the development of robust, scalable, and permanent strategies for CCUS and EOR.

1. Introduction

The escalating threat of climate change has intensified global efforts to reduce atmospheric carbon dioxide (CO_2) emissions, with carbon capture, utilization, and storage (CCUS) emerging as a critical pillar of climate mitigation strategies (Tapia et al., 2018; Chen et al., 2022). Among CCUS pathways, CO_2-enhanced oil recovery (EOR) offers a dual benefit: it improves hydrocarbon extraction from aging reservoirs while sequestering CO_2 in subsurface geologic formations (Melzer, 2012; Hill et al., 2020). This synergy

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addresses both energy security and environmental imperatives, with over millions metric tons of CO_2 already stored globally through EOR operations. However, maximizing the efficiency of CO_2 storage and oil displacement demands a fundamental understanding of the interplay between injected CO_2, reservoir fluids, and complex geologic matrices. As nations strive toward net-zero targets, optimizing CO_2-EOR systems at multiple scales has become a pressing scientific and engineering challenge (Núñez-López and Moskal, 2019).

At the heart of CO_2-EOR and sequestration lie microscopic-scale processes that govern macroscopic outcomes (Du et al., 2024). Pore-scale phenomena-such as CO_2 adsorption onto mineral surfaces, reactive dissolution of carbonate rocks, and capillary-driven multiphase flow in nanometer-sized channels-directly influence reservoir-scale storage capacity, injectivity, and long-term containment (Zhang and Sun, 2021). For instance, CO_2 wettability shifts in hydrophobic shale pores can trap buoyant CO_2 phases, while mineral reactions may either enhance permeability through dissolution or clog pore throats via secondary mineralization. These processes occur across spatial scales spanning angstroms to micrometers and temporal scales from nanoseconds to years, creating a multiscale puzzle that defies intuition (Dehghani et al., 2024). Decoding these mechanisms is essential to predict CO_2 plume migration, prevent leakage, and design injection protocols that balance oil recovery with permanent carbon storage (Mirzaei-Paiaman and Okuno, 2024).

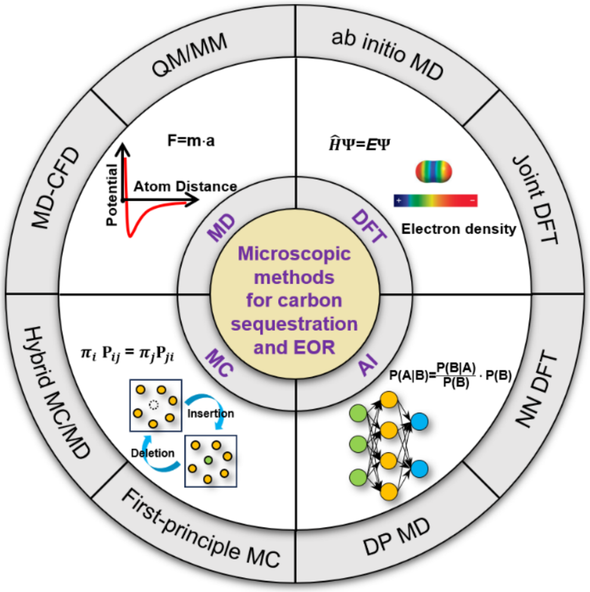

Fig. 1. Typical microscopic methods (middle layers) and cross-methods (outer layer) for carbon sequestration and enhanced oil recovery.

Advancing such knowledge necessitates cutting-edge computational tools capable of resolving atomic-level interactions while bridging to reservoir-scale predictions. Molecular dynamics (MD) simulations unravel the dynamic behavior of CO_2, brine, and oil molecules at interfaces, while density functional theory (DFT) quantifies adsorption energetics and reaction pathways at quantum-mechanical precision. Deep learning (DL) methods accelerate discovery by extracting patterns from vast datasets or surrogate modeling, and Monte Carlo (MC) techniques efficiently sample thermodynamic equilibria in heterogeneous porous media. Together, these paradigms provide complementary lenses to explore the physicochemical complexity of CO_2-reservoir systems, overcoming limitations of experimental techniques in probing confined nanoscale environments. By integrating these approaches (see Fig. 1, researchers can unlock predictive models that inform safer, smarter CCUS deployment in diverse geologic settings.

2. Molecular dynamics (MD) simulations

Molecular dynamics (MD) simulations are a cornerstone of microscopic-scale modeling (Allen and Tildesley, 1987; Liu et al., 2024), leveraging Newtonian mechanics to predict the time-dependent behavior of atoms and molecules within a defined system. By numerically solving equations of motion under empirically derived force fields (such as CLAYFF for clay minerals or INTERFACE FF for interface systems), MD captures the dynamic evolution of molecular interactions. These force fields approximate interatomic potentials, enabling simulations to replicate realistic physicochemical behavior, from bond vibrations to long-range electrostatic forces. The method's reliance on classical mechanics balances computational feasibility with atomic-level resolution, making it uniquely suited to study processes occurring at nanometer scales and picosecond-to-nanosecond timeframes.

MD has been widely applied to investigate CO_2 sequestration and enhanced oil recovery mechanisms. A key focus lies in understanding interfacial phenomena, such as the behavior of CO_2 in brine/oil interfacial region, where MD reveals how CO_2 molecules partition between phases, alter interfacial tension, and influence miscibility. Additionally, MD simulations elucidate diffusion dynamics of CO_2 in nanoporous media, such as shale or clay-rich formations, by tracking molecular trajectories through tortuous pore networks. MD can quantify how confinement and surface chemistry affect transport rates. MD also probes wettability alterations, such as CO_2-induced changes in mineral surface hydrophobicity, and mineral dissolution processes, where acidic CO_2-rich fluids react with carbonate or silicate substrates, altering pore geometry and permeability.

The strength of MD lies in its ability to resolve spatial and temporal details inaccessible to experiments, such as the atomic arrangement at fluid-solid interfaces or the real-time evolution of hydrogen bonding networks. However, its practical utility is constrained by the femtosecond-scale time steps required for numerical stability, limiting simulated timescales to microseconds even with high-performance computing. This restricts direct observation of slow processes like mineral precipitation or macroscopic fluid flow. To address this, researchers often combine MD with statistical sampling or upscaling techniques (Diez, 2024). Case studies highlight these trade-offs: reactive MD simulations of carbonate dissolution, for example, unravel atomic-scale mechanisms of calcite breakdown in acidic CO_2-brine systems, while studies of CO_2 clustering in hydrophobic pores reveal how nanoconfinement promotes phase separation-a critical factor in trapping efficiency. These insights underscore MD's role in bridging molecular interactions to pore-scale reservoir behavior.

The application of MD simulations typically begins with the construction of a representative atomic-scale model of the system under study, such as a CO_2-brine-mineral interface or a nanoporous shale matrix. This involves defining the initial coordinates of molecules (e.g., CO_2, water, oil, and mineral surfaces) within a simulation box, often guided by experimental data. A suitable force field is then selected to describe interatomic interactions, such as CLAYFF for clay minerals or INTERFACE FF for interfacial systems, which governs bonding, van der Waals forces, and electrostatic interactions. Periodic boundary conditions are applied to mimic bulk behavior, and the system is equilibrated through energy minimization and stepwise temperature or pressure regulations (e.g., NVT or NPT ensembles). During the production phase, Newton's equations of motion are iteratively solved to generate trajectories, capturing dynamic processes like adsorption, diffusion, flow, or chemical reactions. Post-simulation analysis tools extract quantitative metrics-such as radial distribution functions, mean squared displacement, or density profiles-to interpret molecular behavior. Validation against experimental data (e.g., adsorption isotherms, contact angles) ensures the reliability of force fields and simulation protocols, enabling predictive insights into subsurface CO_2 behavior.

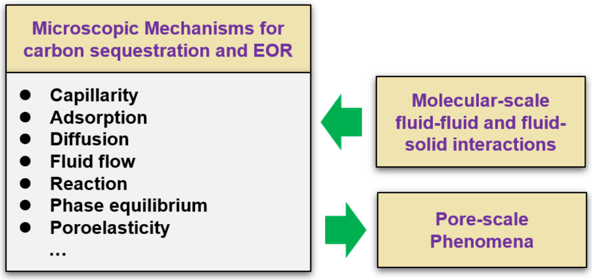

Fig. 2. Microscopic mechanisms for carbon sequestration and enhanced oil recovery.

3. Density functional theory

Density functional theory (DFT) is a general framework and has two variants, namely, electronic DFT and classical DFT. The former models the electronic structure of atoms (Burke and Wagner, 2013; Li et al., 2024), molecules, and materials by solving for the spatial distribution of electron density. And the latter is a statistical mechanics method for properties of inhomogeneous fluids (Lutsko, 2010). The classical DFT is also particularly valuable for modeling fluid–fluid and fluid-solid systems in carbon storage and EOR (Marshall et al., 2012; Camacho et al., 2019). However, we here focus on electronic DFT for simplicity, as it has also been more widely adopted as a basis for developing cross-method approaches. Grounded in the principles of quantum mechanics, electronic DFT bypasses the need to track individual electron wavefunctions, instead using functionals of the electron density to approximate the system's total energy. This approach enables the study of chemical bonding, adsorption phenomena, and reaction mechanisms with high accuracy, making it indispensable for probing interactions at the quantum scale. Unlike classical force fields, DFT inherently accounts for electron exchange and correlation effects, providing a more rigorous framework for predicting bond formation, charge transfer, and surface reactivity.

DFT has proven transformative in studying CO_2 interactions with geologic and engineered materials. A major application lies in calculating adsorption energetics, such as CO_2 binding to mineral surfaces like calcite or kaolinite, or within porous frameworks like metal-organic frameworks (MOFs). These simulations reveal preferential adsorption sites, binding strengths, and the influence of surface chemistry on capture efficiency. DFT also maps reaction pathways for CO_2 mineralization processes, such as the conversion of magnesium oxide (MgO) to magnesium carbonate ($MgCO_3$), by identifying intermediate states, transition barriers, and thermodynamic driving forces. Such insights guide the design of materials that accelerate mineralization, a critical step for permanent CO_2 storage.

The strength of DFT lies in its precision for modeling bond-breaking and bond-forming processes, offering unparalleled resolution of electronic interactions during chemical reactions. However, its computational cost scales steeply with system size, restricting studies to systems containing hundreds of atoms and timeframes limited to static or near-equilibrium states. This precludes direct simulation of dynamic processes like fluid flow or long-term mineral evolution. To mitigate these constraints, DFT is often paired with classical simulations or experimental data. Case studies exemplify its utility: investigations of CO_2 binding at defect sites on mineral surfaces, for instance, demonstrate how vacancies or step edges enhance adsorption, while studies of dopant effects in MOFs reveal how metal substitutions tune pore chemistry to optimize CO_2 selectivity. These atomic-scale insights inform the engineering of next-generation materials for carbon capture and storage.

The application of DFT begins with constructing an atomic model of the system, such as a mineral surface, a MOF, or a reactive interface between CO_2 and a substrate. This involves defining the atomic coordinates of the material, often derived from crystallographic data or simplified representative clusters. A suitable exchange-correlation functional-such as the generalized gradient approximation (GGA) or hybrid functionals-is selected to approximate electron interactions, balancing accuracy and computational cost. The system's electronic structure is then solved iteratively using plane-wave or localized basis sets, optimizing the geometry to minimize total energy and achieve stable configurations. For adsorption studies, CO_2 molecules are placed at various sites on the surface, and their binding energies are calculated by comparing the energy of the adsorbed system to isolated components. Reaction pathways are explored by identifying transition states and intermediates using nudged elastic band (NEB) methods or ab initio molecular dynamics. Post-processing tools analyze charge density differences, partial density of states, and vibrational frequencies to interpret bonding behavior and reactivity. Results are validated against experimental spectroscopic data or thermodynamic measurements, ensuring the model's fidelity in capturing real-world CO_2 interactions. This workflow bridges quantum-scale insights to actionable strategies for improving CO_2 capture and mineralization.

4. Deep learning (DL) approaches

DL leverages artificial neural networks, such as convolutional neural networks (CNNs) and graph neural networks (GNNs) (LeCun et al., 2015; Nagao et al., 2024), to identify complex patterns in data and construct surrogate models that approximate intricate physical relationships. These architectures excel at tasks like regression, classification, and generative design by hierarchically extracting features from structured or unstructured inputs, such as molecular configurations, pore geometries, or simulation outputs. Unlike traditional physics-based models, DL methods learn implicit representations of systems through training on large datasets, enabling rapid predictions of material properties, fluid dynamics, or chemical behavior. This data-driven paradigm has emerged as a transformative tool for accelerating discovery and bypassing computationally expensive simulations.

In CO_2 sequestration and EOR, DL applications span multiple scales and objectives. Neural networks trained on MD or MC data can predict adsorption isotherms or multiphase flow behavior in porous media, reducing reliance on iterative simulations. DL also accelerates quantum-mechanical calculations: frameworks like SchNet and DeepMD replace DFT computations with neural network potentials, retaining quantum accuracy at a fraction of the computational cost. Beyond prediction, DL enables inverse design, where generative models propose novel porous materials, such as MOFs, optimized for high CO_2 uptake by exploring vast chemical spaces beyond human intuition.

The strengths of DL lie in its speed and scalability, particularly for high-dimensional problems where traditional methods falter. Once trained, models can infer results in milliseconds, enabling real-time optimization of injection strategies or material screening. However, these advantages hinge on access to large, high-quality datasets, which are often scarce for complex geologic systems. Additionally, DL models frequently operate as "black boxes," offering limited interpretability into the physical mechanisms driving their predictions. Case studies highlight both promise and challenges: DL-driven discovery of MOFs has identified candidates with record-breaking CO_2 adsorption capacities, while transfer learning techniques adapt models trained on synthetic data to real-world shale systems, mitigating data scarcity. These advances underscore DL's potential to revolutionize subsurface engineering-if paired with robust validation and domain-aware architectures.

5. Monte carlo (MC) methods

MC methods are computational techniques that employ stochastic sampling to explore equilibrium states of a system by generating random configurations weighted by their thermodynamic probabilities (Frenkel and Smit, 2023; Andreeva and Afanasyev, 2024). Unlike molecular dynamics, which tracks time-dependent trajectories, MC focuses on statistical ensembles-such as the grand canonical ensemble (GCMC)-to compute properties like adsorption isotherms or phase equilibria. By iteratively proposing random particle displacements, insertions, or deletions, and accepting or rejecting these moves based on energy criteria (i.e., the Metropolis algorithm), MC efficiently samples the phase space. This approach is particularly powerful for studying systems at thermodynamic equilibrium, where macroscopic properties emerge from averaged microscopic configurations.

MC simulations have become indispensable for modeling gas behavior in complex porous media relevant to CO_2 sequestration and enhanced oil recovery. A prominent application is the study of CO_2/CH_4 competitive adsorption in organic-rich kerogen, where MC quantifies how pore geometry and surface chemistry influence gas selectivity and storage capacity. Additionally, MC elucidates phase behavior in nanopores, such as capillary condensation of CO_2 under confinement, where traditional bulk-phase models fail to capture shifted critical points and confinement-induced hysteresis. These insights are critical for predicting how CO_2 interacts with subsurface matrices under varying pressures and temperatures, directly informing storage site assessments and EOR strategies.

The strength of MC lies in its efficiency for modeling thermodynamic equilibria, especially in systems with complex geometries or low-energy barriers where molecular dynamics struggles to sample rare events. It excels at calculating adsorption isotherms, free energies, and phase diagrams without simulating dynamical processes. However, MC's accuracy depends heavily on the quality of the interatomic potentials used to describe interactions, and it cannot inherently resolve time-dependent phenomena. System sizes are also limited by computational cost, though advanced algorithms like replica exchange mitigate some constraints. Case studies demonstrate MC's utility: simulations of pore-size-dependent hysteresis effects reveal how nanometer-scale variations in shale pores trap CO_2 via capillary forces, while studies of temperature and pressure impacts on storage capacity guide injection protocol optimization. By bridging molecular-scale interactions to reservoir-scale thermodynamics, MC remains a cornerstone of subsurface fluid modeling.

6. Cross-method synergies and challenges

The integration of computational methods unlocks synergies that address individual limitations while amplifying predictive power. For instance, DFT provides quantum-accurate descriptions of adsorption energetics and reaction barriers, which can be combined with DL to parameterize force fields for MD simulations. This DFT-MD coupling ensures that classical models retain quantum-level fidelity when simulating larger systems, such as CO_2 interactions with mineral surfaces or organic matter. Similarly, MC simulations generate vast datasets on thermodynamic equilibria, which train DL models to predict adsorption isotherms or phase behavior, effectively bypassing the need for iterative MC sampling in property prediction. Hybrid workflows, such as embedding DFT-calculated reaction pathways into reactive MD frameworks, enable multiscale modeling of CO_2 mineralization or

Table 1. Parameter settings for eight cases.

Method	Strengths	Limitations
Molecular dynamics (MD)	• Efficient sampling of equilibrium states (e.g., adsorption isotherms). • Captures time-dependent phenomena (e.g., wettabilitys alteration).	(1) Limited to short timescales (nanoseconds to microseconds). (2) High computational cost for large systems. (3) Relies on accurate force fields.
Monte carlo (MC)	• Efficient sampling of equilibrium states (e.g., adsorption isotherms). • Handles complex pore geometries and phase equilibria.	(1) No dynamic/kinetic information. (2) Relies on accurate force fields.
Density functional Theory (DFT)	• Quantum-mechanical accuracy for bond-breaking / formation. • Predicts electronic structure and reaction pathways.	(1) Limited to small systems (100-1,000 atoms). (2) Computationally expensive.
Deep learning (DL)	• Rapid predictions of complex systems (e.g., adsorption isotherms, material properties). • Enables inverse design and surrogate modeling.	(1) Requires large, high-quality training datasets. (2) Limited interpretability (”black-box” nature).
Hybrid / multiscale methods	• Combines strengths. • Bridges multiple scales.	(1) Complex implementation and parameterization. (2) High computational overhead.

brine-rock interactions, bridging electronic-scale chemistry to mesoscale transport phenomena.

Despite these synergies, persistent challenges hinder seamless integration. A critical barrier lies in bridging time scales: MD simulations resolve femtosecond-scale atomic vibrations but cannot directly model hour-long EOR processes like CO_2 plume migration, necessitating statistical extrapolation or coarse-graining techniques. Data scarcity further complicates efforts, as complex geological systems-such as heterogeneous shale matrices or weathered carbonates-lack sufficient experimental or simulation data to train robust DL models or validate MC potentials. Additionally, reconciling computational predictions with experimental observations remains nontrivial. While advanced microscopy, X-ray diffraction (XRD), or spectroscopy provide validation benchmarks, discrepancies often arise from idealized model assumptions or the inability of simulations to fully replicate in situ subsurface conditions.

Addressing these challenges demands interdisciplinary collaboration. For example, machine learning potentials trained on both DFT and MD data could extend the reach of quantum-mechanical accuracy to larger systems, while federated learning frameworks might pool sparse datasets across institutions to enrich DL training. Concurrently, iterative feedback between simulations and experiments-such as tuning force fields against XRD-measured mineral lattice parameters or calibrating DL predictions with microfluidic flow experiments-will tighten the loop between theory and reality. By fostering these cross-method dialogues, researchers can overcome scalability and validation bottlenecks, paving the way for predictive models that reliably guide CO_2 storage and EOR deployment in geologically complex environments.

7. Future directions

1) The next frontier in microscopic-scale modeling lies in developing multiscale frameworks that seamlessly couple MD and MC simulations with reservoir-scale simulators. By integrating atomistic insights into continuum models, researchers can predict CO_2 migration, trapping, and reactive transport across spatial and temporal scales. For example, MD-derived diffusion coefficients or MC-calculated adsorption isotherms could parameterize macroscale flow equations, enabling more accurate forecasts of CO_2 plume behavior in heterogeneous reservoirs. Such frameworks would bridge the gap between pore-scale physics and field-scale engineering, offering a holistic view of CO_2-EOR and storage systems.
2) Algorithmic innovation will further revolutionize computational capabilities. Machine learning potentials, such as neural network-based interatomic potentials (e.g., NequIP), promise to combine the accuracy of quantum-mechanical methods with the speed of classical simulations, enabling larger systems and longer timescales. Active learning strategies could automate the training of these potentials by iteratively selecting optimal configurations for DFT calculations, minimizing computational overhead. Concurrently, adaptive sampling techniques in MD and MC simulations would focus computational resources on rare but critical events, such as nucleation during mineralization or capillary breakthrough in tight pores, enhancing predictive efficiency.
3) Advances in high-performance computing will empower simulations of billion-atom systems, capturing geologic heterogeneity at unprecedented resolution. Exascale plat-

forms could enable real-time modeling of CO_2 interactions in kilometer-scale reservoir models while retaining atomic-level details in critical regions, such as fracture networks or reactive interfaces. Coupled with optimized parallel algorithms, these tools will democratize access to high-fidelity simulations, accelerating the design of tailored CCUS strategies. Finally, the push for open science-through shared databases of molecular models, force fields, and benchmark datasets-will foster reproducibility and collaboration. Community-driven platforms could standardize validation protocols, curate experimental-computational datasets for machine learning, and archive simulations of rare mineralogies or fluid compositions, ensuring that the field advances collectively toward scalable, sustainable carbon management solutions.

8. Conclusion and remarks

The synergistic integration of MD, DFT, DL, and MC methodologies has established a multiscale computational paradigm for deconvoluting the physicochemical mechanisms underlying CO_2 geo-storage and EOR. MD simulations elucidate nanoconfined fluid dynamics through temporal resolution of interfacial phenomena (e.g., contact angle hysteresis, capillary-driven imbibition) and molecular diffusion coefficients under reservoir-relevant conditions. Complementary to this, DFT provides first-principles quantification of adsorption energetics, charge transfer mechanisms, and elementary reaction kinetics at mineral-fluid interfaces. Together, these tools decode the multiscale physics of CO_2-reservoir interactions, from atomic bonding to pore-scale fluid dynamics, providing a foundation to optimize storage security and hydrocarbon recovery.

Realizing this potential demands interdisciplinary collaboration across computational physics, data science, and geochemistry. Bridging the expertise of domain scientists-who define realistic geologic models-with algorithm developers and machine learning engineers will address critical gaps, such as scaling simulations to reservoir-relevant dimensions or interpreting black-box DL predictions. Geochemists and petroleum engineers must further validate models against field data, ensuring computational insights translate to operational guidelines. Only through such synergy can the field overcome persistent challenges like data scarcity, timescale disparities, and the complexity of reactive transport in heterogeneous subsurface systems.

Finally, the future of CO_2-EOR and sequestration lies in model-driven experimental design. Computational insights should guide targeted lab experiments, such as synthesizing materials with DL-predicted pore architectures or testing MD-informed wettability modifiers. Conversely, experimental results must refine simulations, closing gaps in force field accuracy or reaction network completeness. This iterative feedback loop will accelerate the development of robust protocols for CO_2 injection, mineralization, and monitoring, ensuring that subsurface storage is both efficient and permanent. By uniting computation, experimentation, and field deployment, the scientific community can turn theoretical advances into scalable solutions for achieving net-zero emissions.

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Conflict of interest

The authors declare no competing interest.

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