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Invited review

Molecular dynamics insights into wettability-controlled transport in porous media

Ruipeng Lai[1], Yuxiang Nie[1], Xiaoyun Lv[1], Jie Wang[1], Xianyu Song[1]*, Shuangliang Zhao[2]

[1] *Key Laboratory of Water Environment Evolution and Pollution Control in Three Gorges Reservoir, School of Environmental and Chemical Engineering, Chongqing Sanxia University of Science and Technology, Chongqing 404020, P. R. China*

[2] *Guangxi Key Laboratory of Petrochemical Resource Processing and Process Intensification Technology, Guangxi University, Nanning 530004, P. R. China*

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Abstract:
Wettability is a fundamental interfacial property that governs multiphase flow, mass transport, and phase distribution in porous media, thereby influencing hydrocarbon recovery, CO_2 sequestration, shale utilization, and a wide range of subsurface energy systems. Recent developments in molecular dynamics simulations have significantly deepened our understanding of wettability beyond conventional macroscopic phenomena, revealing its molecular basis in surface chemistry, fluid-solid interactions, nanoscale confinement, and interfacial structural ordering. This Review synthesizes recent advances in molecular dynamics studies of wettability in porous media and highlights three emerging directions: (i) The molecular origins, characterization, and material dependence of wettability in heterogeneous porous systems; (ii) wettability-controlled interfacial transport, nanoscale slip, confined phase behaviour, and multiphase displacement across scales; and (iii) multiscale upscaling, data-driven prediction, and the remaining barriers to translating atomistic insights into predictive wettability engineering. It is emphasized that wettability should be regarded as a dynamic and environment-dependent property rather than a static contact-angle metric. Looking forward, the integration of molecular dynamics simulations with multiscale modeling, pore-scale numerical methods, and explainable data-driven approaches is expected to enable predictive wettability engineering in complex porous systems. This review aims to provide a conceptual framework for understanding and controlling interfacial transport in energy-relevant porous materials.

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1. Introduction

Wettability controls phase occupancy, capillary forces, and transport pathways in porous media. By controlling the distribution, displacement, and trapping of immiscible fluids within pore networks, wettability governs residual saturation, phase connectivity, and transport behaviour. In hydrocarbon recovery, CO_2 geological sequestration, shale utilization, and subsurface energy systems, small changes in surface wettability can reorganize fluid configurations and redirect preferential flow paths (Berg et al., 2026). Wettability is therefore not merely a boundary condition, but a design variable for controlling multiphase transport.

Characterizing wettability remains challenging owing to its intrinsically multiscale nature. It reflects the coupled effects of surface chemistry, charge, roughness, pore geometry, fluid composition, pressure, temperature, and nanoscale confinement. Conventional contact-angle measurements on smooth

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*Corresponding author.
E-mail address: diustone@163.com (R. Lai); yxnie25@163.com (Y. Nie); xyl7177@163.com (X. Lv); 13568477984@163.com (J. Wang); xianyusong@sanxiau.edu.cn (X. Song); szhao@gxu.edu.cn (S. Zhao).

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mineral surfaces provide a useful descriptor, but they often fail to represent chemically heterogeneous, rough, and aged pore surfaces. Macroscopic wettability measurements, such as Amott-Harvey and USBM indices, capture averaged wetting states, whereas imaging and microfluidic methods provide improved spatial resolution (Al-Garadi et al., 2022; Mirzaei-Paiaman et al., 2022). Nevertheless, these approaches do not directly resolve the molecular organization and interfacial dynamics governing wetting at solid-fluid and fluid-fluid interfaces. Classical theories such as the Young, Wenzel, and Cassie-Baxter models rationalize apparent wetting states, while pore-scale and continuum models incorporate wettability as an effective input for multiphase transport simulations. Yet these approaches often rely on empirical parameters rather than molecularly derived mechanisms (Sun et al., 2024; Berg et al., 2026). Predictive modeling, therefore, requires a direct connection between surface chemistry, fluid composition, interfacial structure, and transport behavior.

Molecular dynamics (MD) simulations provide this connection by resolving molecular interactions and trajectories at confined interfaces. MD can reveal hydration layers, hydrogen-bond networks, density layering, ion adsorption, oil-component attachment, and nanoscale fluid rearrangement that are inaccessible to most experiments and continuum models (Zhang et al., 2016; Tetteh et al., 2022; Lv et al., 2025). This Review discusses MD insights into wettability-controlled transport in porous media. It covers the molecular origins and characterization of wettability, material- and confinement-dependent wetting behaviour, interfacial transport across surfaces with different wettability, and the upscaling of molecular descriptors to pore-scale and continuum models. The Review also highlights persistent challenges associated with realistic pore representation, force-field accuracy, experimental validation, multiscale coupling, data-driven predictive modelling, and predictive wettability engineering. By linking molecular interfacial mechanisms with cross-scale transport phenomena, this Review provides a framework for moving wettability research from post hoc interpretation towards predictive design.

2. Surface wettability

2.1 MD characterization of wettability

By explicitly recording the motion of atoms and molecules according to interatomic potentials and statistical mechanics, MD provides direct access to molecular arrangements, adsorption configurations, hydrogen-bonding networks, density fluctuations, and interfacial free energy variations, all of which are often difficult to probe experimentally. At the molecular scale, wettability in MD simulations is fundamentally governed by the underlying interatomic potential energy function, which determines the balance of fluid-fluid and fluid-solid interactions. In classical MD, the total potential energy is commonly expressed as:

$$U_t = U_b + U_n \tag{1}$$

where U_t means the total potential energy of the system, U_b stands for the bonded interaction energy (including bond stretching, angle bending, and dihedral torsion terms), and U_n represents the nonbonded interaction energy (e.g., van der Waals and electrostatic interactions) (Rad and Foroutan, 2023). Therefore, the bonded contribution includes bond stretching, angle bending, and dihedral torsion terms, while the nonbonded contribution is typically represented by van der Waals and electrostatic interactions:

$$U_n = \sum_{i<j} \left\{ \underbrace{4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right]}_{\text{Van der Waals}} + \underbrace{\frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}}}_{\text{Electrostatic}} \right\} \tag{2}$$

Here, ε_{ij} represents the summation over all unique particle pairs i and j, σ_{ij} represents the finite distance at which the Lennard-Jones potential becomes zero, r_{ij} denotes the distance between particles i and j, q_i and q_j are the partial charges of particles i and j and ε_0 is the vacuum permittivity constant (Xiang et al., 2026). In wettability simulations, the relative magnitudes of these interaction terms, particularly those between surface atoms and fluid molecules, directly determine interfacial affinity, contact angle, adsorption behavior, and slip transport. Consequently, the predicted wetting behavior is largely contingent on the choice of force field (Jia et al., 2024). MD has been widely applied to interfacial systems in soft matter, materials science, and biology, including nanofluidics and confined-liquid phenomena (Hu et al., 2024, 2025; Yu et al., 2025). These studies have consistently shown that macroscopic wetting and transport behaviours often originate from subtle molecular ordering and localized energetic heterogeneity at solid-liquid interfaces.

2.2 Wettability of mineral-organic surfaces

Guided by these molecular-level interaction principles, MD simulations have increasingly been used to investigate wettability across chemically diverse porous materials. Fig. 1 illustrates the molecular-interfacial coupling framework governing wettability as revealed by MD simulations. Mineralogical diversity, including silica, calcite, clay minerals, and kerogen, plays a key role in surface wettability by modulating surface charge, polarity, and hydrogen-bonding capacity (Zhang et al., 2021; Sanchouli et al., 2024). For example, clay basal surfaces exhibit strong anisotropic wettability due to their layered structures and ion exchange effects (Zhang et al., 2016), while kerogen surfaces display pronounced hydrophobicity linked to aromatic and aliphatic domains (Sanchouli et al., 2024). At the molecular scale, these compositional differences translate into distinct fluid-surface interaction mechanisms. (Cui et al., 2022) revealed the importance of molecular composition in influencing nanoscale oil-matrix interactions and interfacial wettability in shale reservoirs by modelling the wetting of shale-oil nanodroplets on minerals and organic matter in various environments.

Beyond intrinsic composition, external physicochemical conditions dynamically modulate these interactions and thus wettability. The adsorption of organic components, such as asphaltenes, can significantly shift surfaces from water-wet to oil-wet states by modifying interfacial energy and blocking polar sites. Similarly, surfactants and organosilanes can induce

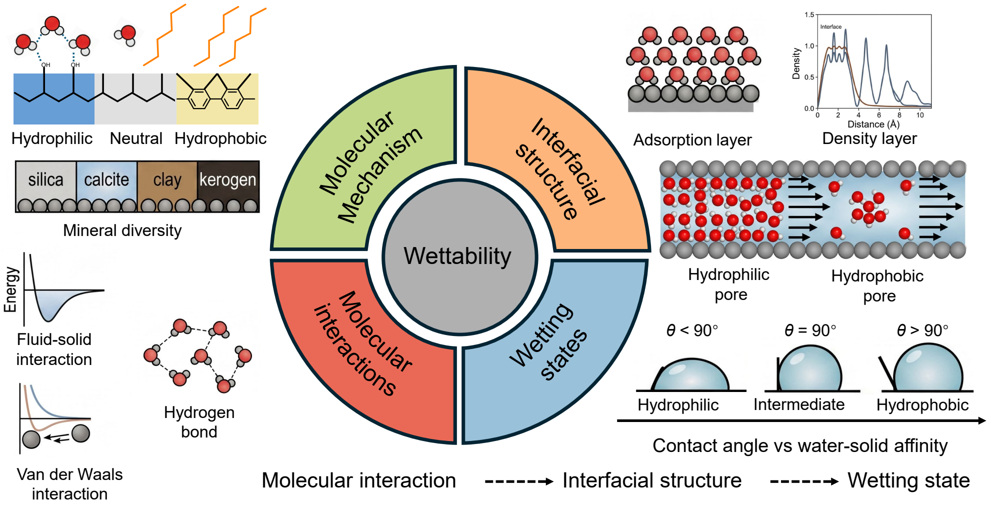

Fig. 1. Molecular-interfacial coupling framework governing wettability.

controlled wettability alteration via molecular adsorption and reorganization at interfaces (Tetteh et al., 2022). Notably, gas pressure variations have also been shown to dynamically alter wettability by influencing fluid density and adsorption equilibria at solid surfaces (Guo et al., 2026). As illustrated in Fig. 2, CO_2 flooding and CO_2 huff-n-puff (HNP) in a shale calcite dead-end nanopore produce distinct fluid configurations, potential-energy evolution, and axial CO_2 migration velocities, highlighting how confinement and injection mode regulate competitive adsorption and displacement. These findings challenge the classical view of wettability as a static property and instead establish it as a dynamic, environment-dependent molecular phenomenon, governed by competing interfacial interactions and nanoscale confinement effects. Table 1. summarizes the MD-based methods for contact-angle characterization and compares their applicability across different wettability studies.

2.3 Material- and environment-dependent contact-angle landscapes

Wettability in porous media is material-dependent, but it is not a fixed material property. MD studies reveal broad wetting diversity across representative mineral and carbonaceous surfaces. Hydroxylated silica and quartz are generally water-wet, whereas clay minerals display termination- and cation-dependent wettability. Calcite frequently shifts towards oil-wet conditions in the presence of polar hydrocarbons or specific brines. Graphitic carbon is typically hydrophobic, while graphene oxide exhibits chemically tunable wettability. Kerogen, coal, and shale organic matter show substantial variability associated with maturity, aromaticity, and heteroatom composition. These trends provide useful reference states, but the reported contact angles should be interpreted as condition-dependent ranges rather than intrinsic constants (Xin et al., 2025).

In Table 2, the broad contact-angle ranges compiled reflect the inherently condition-dependent nature of wettability. Here, θ_{MD} denotes the contact angle derived from molecular dynamics simulations. This variability becomes even more pronounced when fluid molecules are confined within pore structures of finite geometry. Beyond surface chemistry, confinement and pore geometry can substantially reshape wetting behaviour. In slit pores, nanopores, and pore throats, fluid molecules experience overlapping solid-fluid interactions from opposing walls. This produces density layering, preferential molecular orientation, modified hydrogen-bond networks, and altered diffusion near the interface (Qin et al., 2024). As pore size approaches molecular dimensions, wetting is increasingly governed by molecular packing, adsorption-desorption kinetics, and interfacial friction rather than by bulk capillarity alone. Curvature, roughness, and chemically patchy walls further introduce contact-line pinning, heterogeneous slip, and local energy barriers, making the apparent contact angle scale- and geometry-dependent (Chu and Zhang, 2025).

Environmental conditions add another level of regulation. Temperature changes hydrogen-bond stability, viscosity, and interfacial free energy (Shu et al., 2022). Pressure modifies fluid density, adsorption, and phase behaviour. Salinity and ion identity control charge screening, ion bridging, and hydration structure at mineral surfaces. In CO_2-brine, oil-water, and gas-water systems, competitive adsorption among fluids and solutes can reorganize interfacial layers and shift local wetting states during transport. Thus, wettability in confined porous media is best understood as a responsive interfacial state determined jointly by material chemistry, pore geometry, and fluid environment. Consequently, a single contact angle cannot fully represent wettability in heterogeneous nanoporous systems. A more informative description should report the material surface, pore geometry, fluid composition, thermodynamic conditions, and MD protocol together with molecular descriptors such as adsorption energy, density layering, residence time, diffusion coefficient, and interfacial friction. This Review provides the necessary bridge from static wettability characterization to dynamic interfacial transport.

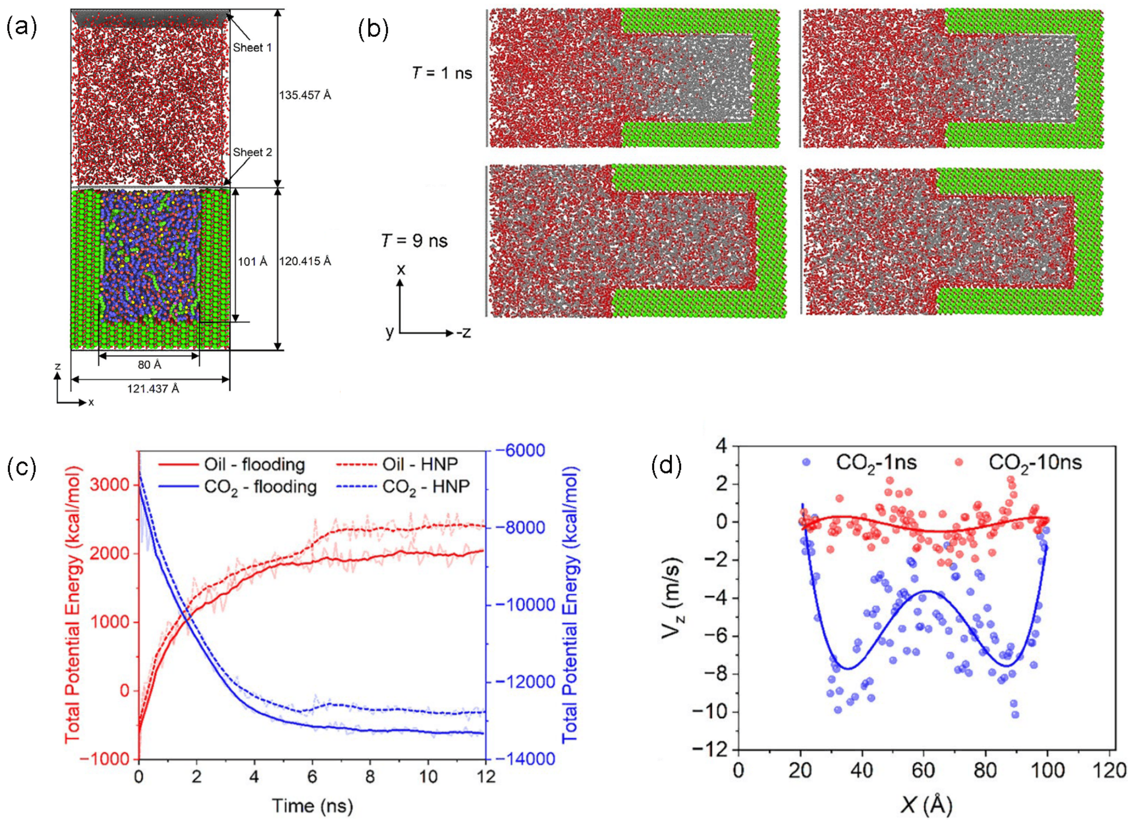

Fig. 2. (a) Initial configuration of the simulation model, (b) snapshots in the *x*-*z* plane showing CO_2 flooding and CO_2 HNP processes at 1 ns and 9 ns in a shale calcite dead-end nanopore, (c) evolution of total potential energy of CO_2 and oil during the CO_2 flooding and CO_2 HNP processes and (d) CO_2 migration velocity along the *Z*-axis during CO_2 HNP. Color code: Gray, carbon atoms and all hydrocarbons; red, oxygen atoms, modified from Guo et al. (2026).

2.4 From static wettability to dynamic interfacial behavior

Although contact angle provides a convenient classification of wetting states, it is an incomplete predictor of transport in confined pores. Surfaces with nearly identical apparent contact angles can differ substantially in adsorption strength, slip length, interfacial friction, residence time, and displacement efficiency, because these properties are governed by near-wall molecular ordering, density layering, and energy dissipation rather than by static interface geometry alone. For instance, the slip length of water in hydrophilic nanopores is determined by the density distribution within the interfacial contact layer, not by the macroscopic contact angle (Lv et al., 2025). Similarly, a universal scaling relationship between diffusion and wetting free energy has been observed across chemically diverse surfaces, reinforcing the view that molecular mobility is not uniquely determined by a single contact-angle value (Agosta and Dzugutov, 2026). Transport in wettability-controlled pores emerges from coupled diffusion, adsorption-desorption kinetics, capillary invasion, contact-line motion, phase exchange, and fluid-solid friction. Under nanoconfinement, surface chemistry reshapes hydration structure and density layering, thereby modulating slip, molecular mobility, and multiphase displacement. Dynamic wettability is therefore best understood not as a time-varying contact angle, but as an environment-responsive interfacial state that depends on flow, pressure, composition, and confinement. This Review shifts the emphasis from static angle measurement to the molecular descriptors that directly control transport, providing the conceptual bridge from wettability characterization to the analysis of wettability-controlled transport mechanisms developed in the sections that follow.

3. Wettability-controlled transport across scales

3.1 Interfacial transport under different wettability conditions

In fact, wettability is not merely an interfacial property but a key regulator of fluid transport, phase distribution, and mass transfer in porous media. MD simulations also provide detailed insight into nanoscale transport mechanisms, which serve as the foundation for understanding macroscopic flow behavior. At the nanopore scale, wettability strongly influences fluid structuring and mobility. In hydrophilic systems, water molecules form stable adsorption layers on mineral surfaces, reducing effective pore space and hindering non-wetting phase transport (Zhao et al., 2017). In contrast, hydrophobic conditions promote slip flow and reduce viscous resistance, leading to enhanced transport efficiency (Zhao et al., 2017). These effects are further modulated by the pore size, with smaller pores exhibiting stronger confinement-induced deviations from

Table 1. MD methods for contact-angle characterization in porous-media wettability studies.

Method	Typical systems	Strengths	Main limitations	Reference
Sessile droplet	Flat mineral, carbon, and organic surfaces	Experimental analogue; simple geometry	Finite-size effects; line tension; baseline choice	Zhang et al. (2016)
Cylindrical droplet	Periodic slit pores and nanochannels	Lower curvature artefacts; improved sampling	Requires lateral homogeneity	Zhao et al. (2017)
Density contour fitting	Conventional droplet and confined-fluid simulations	Automated interface detection	Threshold and smoothing dependent	Tetteh et al. (2022)
Circle/spherical-cap fitting	Smooth homogeneous surfaces	Simple; widely comparable	Fails for small droplets, distorted interfaces, and strong heterogeneity	Sanchouli et al. (2024)
Young-equation route	Thermodynamic wettability analysis	Direct link to surface free energy	Difficult solid–liquid free energy; model-dependent	Chowdhury et al. (2026)
Dynamic contact angle	Dynamic wetting and displacement processes	Captures hysteresis and nonequilibrium wetting dynamics	Sensitive to forcing, timescale, and equilibrationand equilibration	Sun et al. (2024)

Table 2. Summarizes representative wettability characteristics of typical porous-media materials and the main factors responsible for variations in MD simulations.

Material surface	Interface conditions	Key condition	θ_{MD} wetting state (°)	Reference
Pyrophyllite	Gas/Liquid/Solid	Pressure	90-150	Ho and Wang (2021)
Kaolinite	Liquid-Solid	Basal/edge surface, cations	0-105	Shi et al. (2023)
Calcite	Brine–oil/surfactant systems	Facet, ions, oil polarity	90-130	Tetteh et al. (2022)
Graphene/graphite	Liquid-Solid	External tension, geometry	0-68.5	Kateb and Isacsson (2023)
Graphene oxide	Liquid-Solid	O/C ratio	20-100	Wei et al. (2014)
Kerogen/organic matter	Liquid-Solid	Droplet size, heteroatom content	65-75	Sanchouli et al. (2024)
Coal/SiO_2	Liquid-Solid	Rank, minerals, functional groups	58.5-130.6	Chen (2025)
Functionalized polymer	Water/oil/brine	Functional groups, crosslinking	0-80	Mirzaalipour et al. (2024)

continuum behavior (Jia et al., 2025). Non-equilibrium MD simulations have demonstrated that water transport through carbon nanotube membranes is strongly governed by tube flexibility, surface wettability, and pore size distribution, thereby enabling the establishment of a quantitative framework capable of predicting experimentally observed flux enhancement (Liu et al., 2024). Importantly, such transport behaviours fundamentally originate from molecular-level variations in interfacial interactions. Wettability heterogeneity has been shown to arise from differences in surface charge distribution, hydrogen bonding, and interfacial energetics (Chowdhury et al., 2026). Similarly, our previous work revealed that nanosized water droplets can spontaneously self-propel on a MoS_2/graphene heterojunction surface driven by wettability differences, while inter-droplet hydrogen-bond interactions further enhance propulsion velocity (Hu et al., 2022).

3.2 Confined nanoscale transport in slit pores and nanopores

To elucidate the mechanistic roles of wettability and confinement in nanoscale transport, MD simulations of a graphene-like slit-pore flow model were conducted to systematically investigate nanoconfined liquid transport under varying surface wettability and pore confinement conditions (Zhao et al., 2017), as shown in Fig. 3(a). As observed in Fig. 3(b), a distinct quantitative relationship between the contact angle and the wetting parameter α_w was observed, suggesting that a decrease in wall-fluid interaction strength causes a progressive increase in contact angle, i.e., a change from wetting/solvophilic to non-wetting/solvophobic surfaces. Beyond this static wettability property, transport behavior is critically governed by interfacial slip and confinement effects. As shown in Fig. 3(c), the slip length is directly correlated with pore width and increases substantially under strong

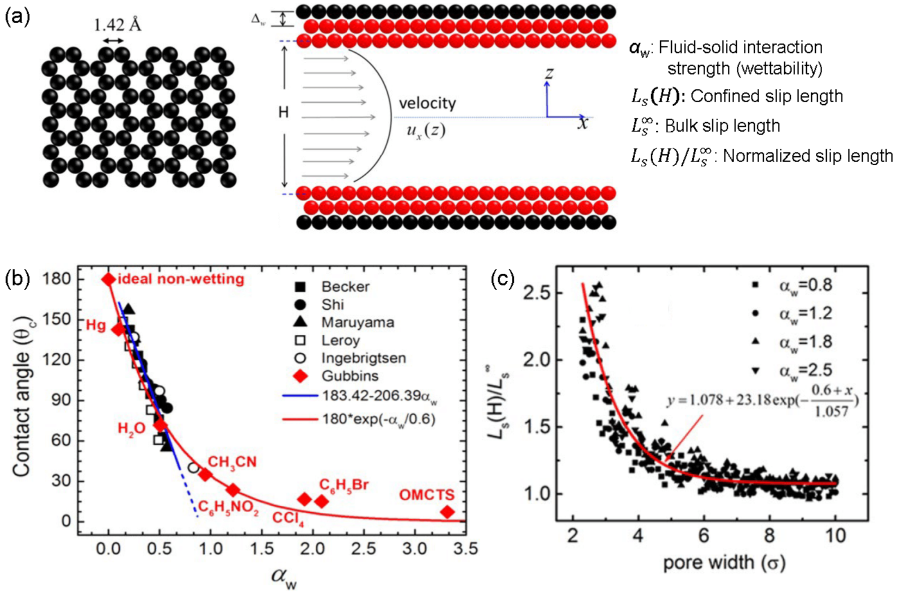

Fig. 3. (a) Schematic illustration of fluid flow in a slit pore composed of graphene-like layers, where the black layers represent pristine graphene walls, (b) relationship between contact angle and wetting parameter and (c) dependence of reduced slip length on pore width, modified from Zhao et al. (2017).

confinement, particularly for weakly wetting surfaces. As the pore width decreases to only a few molecular diameters, the slip length (L_s) increases sharply, demonstrating that nanoscale confinement enhances interfacial slippage rather than merely reflecting a surface property. More fundamentally, the water slippage at solid surfaces is governed primarily by the density distribution roughness of the interfacial contact layer, rather than by surface wettability itself, thereby providing a more fundamental molecular property for predicting slip behavior (Fang et al., 2025; Lv et al., 2025).

This mechanism highlights that flow enhancement in nanoconfined systems arises from coupled interfacial and confinement effects. In line with this, Classical Murray's law has been generalized for nanoscale fluid transport through the incorporation of interfacial slip and confinement-induced fluid-property variations, leading to a generalized resistance-matching principle for hierarchical nanomaterial design (Cao et al., 2026). They also revealed that nanoconfined flow enhancement cannot be attributed to wettability alone, but instead arises from the coupled effects of reduced interfacial friction and confinement-strengthened slip in graphene-like slit pores (Chen et al., 2024). Extending from static to dynamic perspectives, recent studies further reveal that wetting-transport coupling is intrinsically a non-equilibrium process. Diffusion and wetting are intrinsically coupled, with molecular diffusion governing interfacial mass redistribution and energy dissipation, thereby regulating wetting kinetics, spreading dynamics, and interfacial stability (Agosta and Dzugutov, 2026). Accordingly, dynamic wettability-transport coupling involves co-evolving interfacial structure, energy dissipation, and mass transport, which can be effectively captured by non-equilibrium MD. For example, enhanced wettability has been shown to promote low-frequency phonon coupling, thereby strengthening interfacial heat transfer at Fe nanoparticle-water interfaces. However, translating these nanoscale insights to realistic porous media remains challenging. In real systems, mineralogical heterogeneity, surface roughness, organic-inorganic coupling, and pore-network disorder lead to spatially non-uniform interfacial structures, causing local variations in slip, capillary resistance, and permeability across the pore network.

3.3 Wettability-controlled transport in porous systems

MD applications in representative porous systems show that wettability regulates not only local wetting preference but also phase stability, competitive adsorption, interfacial transfer, and confined transport. These effects are particularly evident in CO_2-water-mineral systems, hydrate-bearing nanopores, organic-rich shale pores, and hydroxylated oxide interfaces, where molecular-scale changes in interfacial ordering and mobility can be amplified into distinct phase and transport behaviours. For instance, CO_2-water wettability in silica nanopores affects thin film stability, capillary pressure, and dissolution kinetics (Sun et al., 2024). As shown in Fig. 4, changes in wettability also alter the relationship between scCO_2 saturation and specific interfacial area, and lead to distinct scCO_2 cluster-size distributions during pore-scale evolution, indicating that wetting conditions directly regulate phase connectivity and interfacial configuration. Similarly, wettability governs the nucleation and stability of CO_2 hydrates, where hydrophilic surfaces stabilize water-rich phases while hydrophobic environments favor gas aggregation (Jia et al., 2025). At the molecular scale, these effects originate from changes in interfacial structure and dynamics. For example, the transition from low to high wettability is essentially a surface-induced phase transition in the interfacial contact

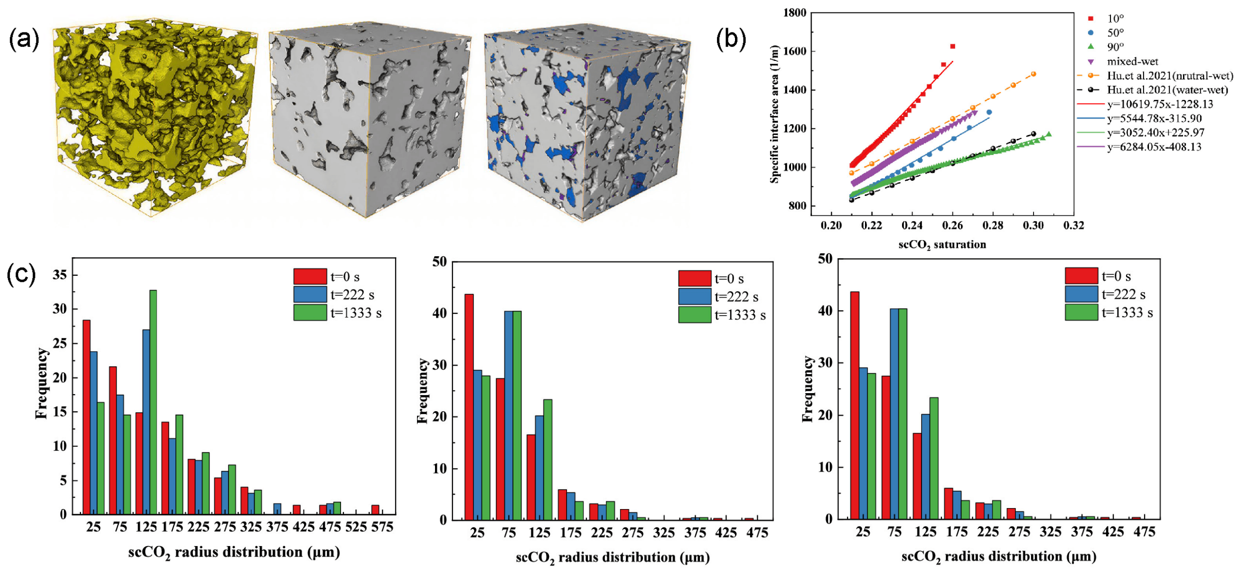

Fig. 4. (a) Simulation domain showing (left) the pore space, (middle) the single-wet sample, and (right) the mixed-wet sample, (b) evolution of $scCO_2$ saturation as a function of specific interfacial area under four wettability conditions and (c) $scCO_2$ cluster-radius distributions at $t = 0$, 222, and 1,333 s for strongly water-wet, weakly water-wet, and intermediate-wet samples, shown from left to right, modified from Sun et al. (2024).

plane, where changes in molecular ordering and diffusivity are intimately linked to the wetting state (Chowdhury et al., 2026). Wettability in three-phase systems depends strongly on interfacial chemistry and the balance between van der Waals and electrostatic interactions, while temperature and oil-water coexistence alter hydrogen-bonding networks at the surface, thereby modulating wetting behavior (Xu et al., 2026).

These molecular interactions further translate into coupled phase-transport behaviours under confinement. For example, moisture diffusion, vapor condensation, and infiltration processes are strongly dependent on wettability and pore confinement (Hu et al., 2019). Gas-enhanced methane recovery in graphene nanoslits is governed by confinement-dependent adsorption and competitive displacement, with CO_2 exhibiting the strongest adsorption and thus the greatest potential to displace adsorbed CH_4 under identical conditions (Bekeshov et al., 2023). Collectively, these MD studies highlight that wettability is not merely an isolated surface characteristic, but a key molecular property governing the coupled evolution of phase behaviour, interfacial organization, and transport dynamics under nanoscale confinement.

3.4 Bridging molecular-scale wettability and multiscale transport modelling

MD resolves the molecular origins of wettability, but its intrinsic limitations in length and time scales prevent the direct simulation of transport in realistic pore networks. Its broader value, therefore, lies in providing molecular-scale interfacial and transport parameters for larger-scale models (Wang et al., 2026), including contact angle, interfacial tension, adsorption energy, diffusivity, slip length, and interfacial friction. Across multiscale modelling approaches, including coarse-grained simulations, lattice Boltzmann method and phase-field methods, pore-network modelling, computational fluid dynamics, and data-driven frameworks, MD-derived interfacial and transport properties are increasingly incorporated into larger-scale transport models. These molecular-scale quantities serve as constitutive inputs or boundary conditions for predicting multiphase invasion, phase connectivity, trapping, dissolution kinetics, and displacement efficiency. For example, MD-derived wettability parameters were used in a lattice Boltzmann model to simulate dynamic CO_2 dissolution in three-dimensional porous media, accurately reproducing experimental dissolution patterns across a range of wetting conditions (Sun et al., 2024). Similarly, MD-informed slip lengths and adsorption isotherms have been used to improve pore-network and computational fluid dynamics predictions for membrane separation (Chen et al., 2024) and mineral dissolution in shale (Zhao et al., 2026). This multiscale integration bridges molecular interfacial physics, pore-scale flow organization, and continuum-scale transport.

4. Challenges and future directions

Despite substantial progress in elucidating the molecular origins of wettability through MD simulations, achieving truly predictive and controllable wettability in porous media systems remains a formidable challenge. This difficulty arises from the intrinsic multiscale nature of wettability, which is simultaneously governed by molecular interactions, surface chemistry, pore geometry, fluid composition, and evolving thermodynamic conditions. As a result, several critical challenges remain in achieving predictive and controllable wettability in porous media systems.

1) A major limitation lies in the absence of robust multiscale frameworks capable of bridging MD simulations with pore-scale and reservoir-scale models. Specifically, key

challenges include the scale mismatch between nanoconfined interfacial properties and pore-scale flow, the lack of transferable descriptors linking molecular interactions to effective wettability parameters, and inconsistent boundary conditions across scales. Thus, future efforts should focus on physics-informed upscaling, including deriving MD-based constitutive relationships (e.g., contact angle-surface energy mappings) and embedding them into pore-scale models (e.g., lattice Boltzmann method or phase-field methods), alongside integrating MD-derived descriptors into mesoscale frameworks.

2) Another key challenge is that many current MD studies still rely on simplified systems with idealized pore geometries and chemically homogeneous surfaces. Specifically, the lack of realistic surface reconstruction, the limited representation of mixed mineral/organic compositions, and the neglect of spatially varying interaction potentials hinder the transferability of MD results to real systems. Innovations in digital-rock reconstruction, surface-aware molecular modelling, and hybrid simulation approaches may provide more realistic and transferable descriptions of such complex environments. Integrating high-resolution imaging with atomistic model construction, employing spatially resolved or reactive force fields, and coupling MD with pore-scale methods can enable a more realistic representation of heterogeneous porous systems.
3) In addition, most existing studies emphasize static wettability properties, whereas real interfacial systems often undergo dynamic and non-equilibrium wettability evolution driven by changes in pressure, temperature, salinity, and chemical reactions. Key limitations include the inability of equilibrium MD to capture transient contact-line dynamics, interfacial restructuring, and transport-driven wettability transitions under external gradients. Capturing these transient processes will require broader adoption of time-resolved, reactive, and non-equilibrium MD methods capable of resolving wettability evolution beyond equilibrium states. In particular, non-equilibrium MD with imposed gradients, reactive MD for surface evolution, and MD-data-driven hybrid models offer promising routes for capturing dynamic wetting-transport coupling.
4) Finally, the integration of data-driven methods and explainable machine learning presents a promising frontier for wettability research. Future studies should focus on standardized MD-derived descriptor databases, structure-wettability surrogate models for the direct prediction of macroscopic parameters, and the incorporation of physical constraints (e.g., thermodynamic consistency) into machine-learning architectures. In particular, unsupervised learning approaches, including clustering and Gaussian mixture models, may help uncover distinct wettability regimes, interfacial states, and phase behaviours by mapping high-dimensional MD features into low-dimensional, physically interpretable phase spaces that are otherwise difficult to resolve through manual interpretation alone.

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Conflicts of interest

The authors declare no competing interest.

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