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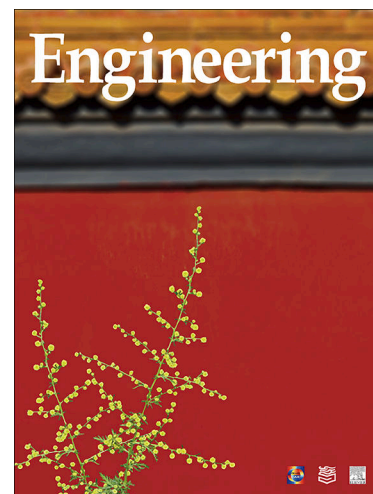
Integrating Omics Concept into Asphalt Science: Current Applications and Emerging Opportunities

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Civil Engineering Materials—Review

Integrating Omics Concept into Asphalt Science: Current Applications and Emerging Opportunities

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ABSTRACT

Asphalt omics is an emerging interdisciplinary field that integrates biology, materials science, computational science, and transportation science to address the complex properties of asphalt and the growing volume of high-throughput

testing data. This study traces the early adoption of omics concepts in asphalt research, including asphalt fingerprinting, fractionation, and mixture design programming. It then outlines the core components of the asphalt omics framework, which operates across three levels: asphalt material, pavement, and environmental omics. Furthermore, a systematic architecture for asphalt omics is presented, comprising testing, analysis, and data platforms. Leveraging omics principles, this study examines the integration of multiscale asphalt information through advanced characterization techniques, the application of artificial intelligence for efficient data processing, and the development of a comprehensive smart asphalt omics database. As a transformative research paradigm, asphalt omics provides a data-driven approach that bridges empirical, theoretical, experimental, and practical insights, thereby accelerating the development of multifunctional asphalt materials, high-performance pavements, and sustainable road transportation.

1. Introduction

Genomics has emerged as a transformative research paradigm, grounded in the methodologies and technologies developed during the Human Genome Project [1]. Omics refers to a systematic scientific approach that employs high-throughput testing, intelligent analysis, and database construction to study all components within specific layers to elucidate their structures, functions, interactions, and dynamic changes from a comprehensive and integrated perspective, thereby capturing system complexity beyond isolated molecular events. For example, genomics enables comprehensive decoding of gene sequences and regulatory networks, providing system-level insights into biological functions. Recognizing the limitations of single-omics studies in capturing complex systems, multi-omics frameworks have been developed to integrate diverse datasets and deepen mechanistic understanding [2].

Omics technologies have since expanded beyond the life sciences, driving transformative advances across multiple disciplines [3]. In biomedicine, omics underpin precision medicine, enhancing cancer detection, diagnosis, and treatment using large-scale cancer datasets [4]. Pharmacology and toxicology leverage omics-driven databases to predict drug responses and optimize therapies. In food science, omics enhances food safety, quality control, and traceability [5]. Environmental sciences utilize omics technologies to elucidate biological responses to environmental stressors and uncover links between ecosystem dynamics and human health. These examples highlight the broad applicability of omics technologies in addressing complex scientific challenges. Asphalt omics is an interdisciplinary approach inspired by biological omics, which conceptualizes the microscopic components governing asphalt performance as fundamental functional units. It utilizes high-throughput testing and intelligent data processing to comprehensively analyze data from a unified perspective. Asphalt omics encompasses elemental composition analysis, chemical bond characterization, molecular structure modeling, microstructural simulation, macroscopic performance evaluation, and environmental responsiveness. By elucidating how these functional units collectively influence asphalt performance, asphalt omics systematically reveals the interactions among asphalt composition, microstructure, macro-performance, and environmental impacts. As a branch of materials omics, asphalt omics leverages established omics methodologies and integrates advanced material design strategies to expedite the entire process from material discovery to application. Research initiatives in China, the United States, Japan, and the European Union have adopted omics-based strategies for rapid material development, resulting in significant advancements in fields, such as electronics, energy, and aerospace. In road engineering, understanding the relationship between the material composition and pavement performance remains a critical research priority. Unlike conventional empirical or trial-and-error methods, asphalt omics emphasizes the precise identification and manipulation of functional units, enabling rational, data-driven material design and driving a paradigm shift in asphalt material research. Driven by advances in characterization technologies and intelligent data analytics, asphalt omics accelerates the identification of critical functional units and elucidates their mechanisms, deepening our understanding of the interrelationships among asphalt composition, microstructure, macro-performance, and environmental impacts. This approach established a comprehensive framework for data-driven material design and sustainable pavement development. First, this study examines the early adoption of omics concepts in asphalt research, such as fingerprinting, component analysis, and mixture design programming. Subsequently, a three-level framework encompassing material, pavement, and environmental omics was proposed. Finally, the core

infrastructure supporting asphalt omics, which comprises testing, analysis, and data platforms, is discussed. Furthermore, this study outlines a systematic paradigm for multidimensional asphalt omics to guide future innovations in road materials and engineering by introducing advanced testing technologies and artificial intelligence (AI)-driven analytical and enhanced asphalt-related databases.

2. Preliminary adoption of asphalt omics

The foundational principles of asphalt omics have been implicitly presented in decades of asphalt research. Methods, such as asphalt fingerprinting, chemical fractionation, and mixture design programming, demonstrate an omics-oriented approach by emphasizing component identification, composition–property relationships, and data-driven design. As shown in Fig. 1 [6–11], these methods represent the early adoption of omics thinking in asphalt science, although historically applied in a fragmented manner without a unified framework. For further details, including principles, methodologies, and examples, refer to the Sections S1–S3 in Appendix A.

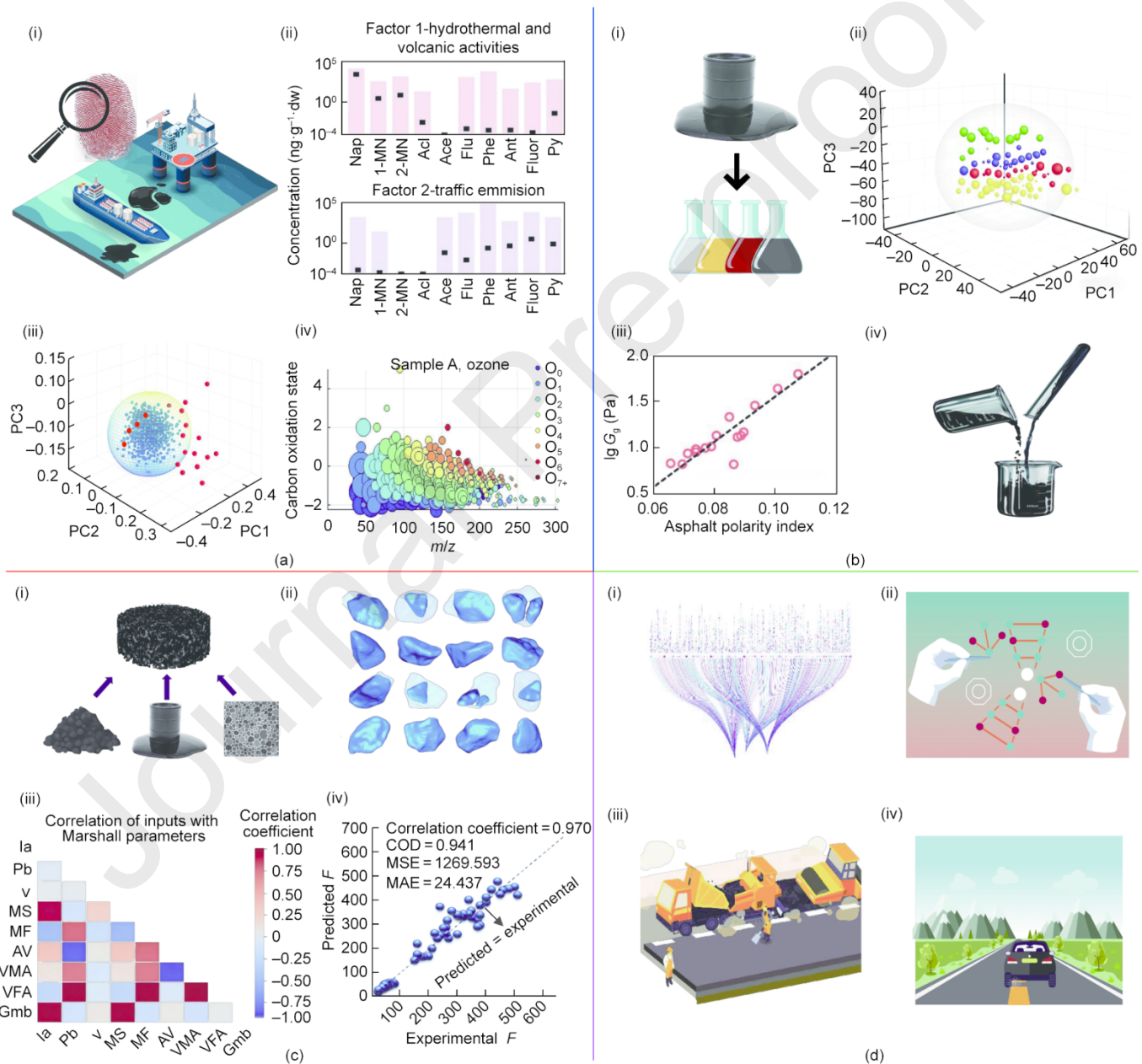


Fig. 1. Adoption of omics concepts in asphalt science. (a) Asphalt fingerprint: (i) chemical characterization, (ii) source identification, (iii) property prediction, and (iv) environment evaluation. (b) Asphalt fractionation: (i) component

separation, (ii) primary distillation, (iii) property correlation, and (iv) asphalt blending. (c) Mixture design: (i) material prop

data-driven integration, (ii) material design, (iii) pavement construction, and (iv) road sustainability. Nap: naphthalene; 1-MN: 1-methylnaphthalene; 2-MN: 2-methylnaphthalene; Acl: acenaphthylene; Ace: acenaphthene; Flu: fluorene; Phe: phenanthrene; Ant: anthracene; Fluor: fluoranthene; Py: pyrene; dw: dry weight; PC1, PC2, and PC3 denote the first, second, and third principal components derived from principal component analysis (PCA), respectively; G_g denotes the glassy dynamic modulus at extremely high frequency (low temperature); G_{mb} denotes bulk specific gravity of the mixture. VFA: voids filled with asphalt; VMA: voids in mineral aggregate; AV: air voids; MS: Marshall stability; MF: Marshall flow. Pb represents binder content; Ia is the aggregate index which denotes the particle shape and texture characteristics of aggregates; ν is the viscosity of the bitumen; F denotes the predicted target Marshall mix design parameter; COD represents the coefficient of determination; MSE and MAE represent the mean squared error and mean absolute error, respectively. Reproduced from Refs. [6–11] with permission.

2.1. Asphalt fingerprints

Asphalt fingerprinting employs high-throughput analytical techniques to capture the unique chemical signatures of asphalt samples, facilitating source identification, performance prediction, and environmental assessment (Fig. 1(a)). From an omics perspective, fingerprinting generates comprehensive molecular profiles that underpin integrated analyses and functional unit identification. Further details are provided in Section S1.

2.2. Asphalt fractionation

Asphalt fractionation separates asphalt into distinct chemical groups, clarifying the contributions of specific molecular domains to macroscopic properties and supporting composition–property modeling (Fig. 1(b)). From an omics perspective, fractionation elucidates how component units collectively influence material performance and enables integrated analysis. Additional information is available in Section S2.

2.3. Asphalt mixture design programming

Asphalt mixture design programming utilizes data-driven methods for mixture composition optimization and performance prediction, providing a systematic framework for material design (Fig. 1(c)). From an omics perspective, this approach treats mixture parameters as programmable elements that can be quantitatively linked to material behavior. Section S3 contains further details.

2.4. Asphalt omics

Asphalt omics, inspired by omics approaches in life sciences and grounded in the petroleomics paradigm, seeks to systematically decode complex structure–function–performance relationships within asphalt systems [12] (Fig. 1(d)). Asphalt omics, analogous to multi-layer integration in biological research, unifies multiscale data from diverse analytical techniques within a comprehensive framework. This framework is anchored by three core technological platforms—high-throughput testing, intelligent analysis, and smart databases—and encompasses three interrelated levels: asphalt material, pavement, and environmental omics (Fig. 2).

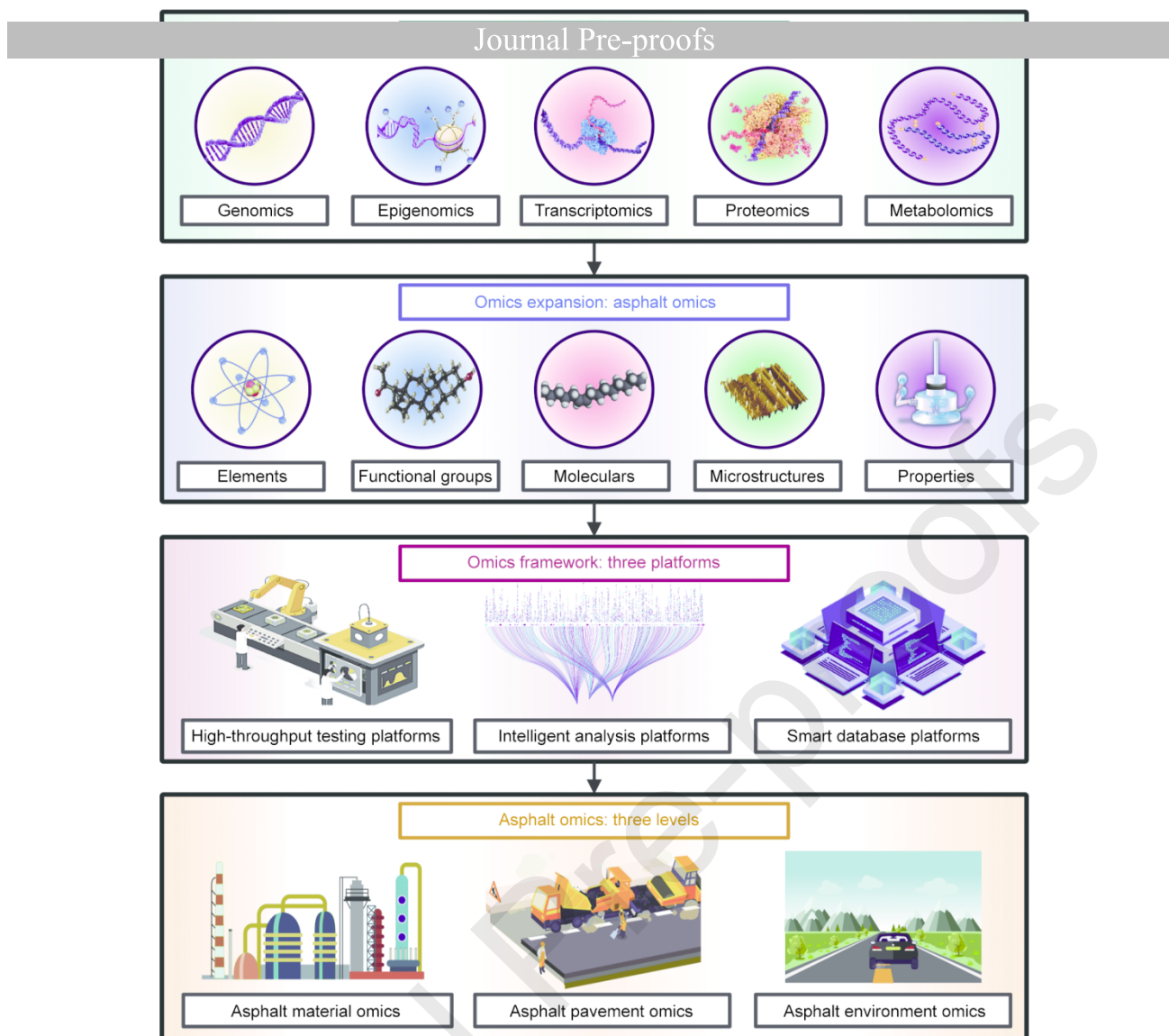


Fig. 2. Framework of asphalt omics: integration of three technological platforms across three levels.

(1) **Asphalt material omics.** This level investigates the relationship between the microscopic composition and macroscopic properties. High-throughput, precision testing enables detailed characterization of complex chemical and physical structures, elucidating the impact of molecular features on key properties, such as rheological behavior and durability [13]. The integration of AI and simulation tools facilitates the extraction of composition–structure–property relationships from large datasets, supporting the proactive design of high-performance asphalts and alternative materials. Expanding asphalt databases further accelerates predictive modeling.

(2) **Asphalt pavement omics.** This level connects material properties, design parameters, and construction practices to pavement performance. Critical factors, such as binder type, aggregate morphology, gradation, and volumetric properties, along with production parameters, such as mixing, paving temperatures, and compaction, significantly influence outcomes [14]. Machine learning (ML) and structural modeling establish quantitative relationships among these variables, thereby enhancing prediction and process optimization. Incorporating monitoring data supports the development of maintenance strategies and improves the long-term performance of asphalt pavements.

(3) **Asphalt environmental omics.** This level addresses the environmental impacts across the asphalt lifecycle [15]. Pavements incorporating chemical modifiers or waste materials can accelerate the release of pollutants, such as volatile organic compounds (VOCs), particulate matter, and heavy metals—particularly under high temperatures. Databases

correlating traffic volumes with pollution levels enhance the environmental omics framework [16]. Integrating monitoring data and health assessments within road zones enables the identification of pollution sources, emission tracking, impact prediction, and supports the adoption of low-emission materials and economically friendly technologies.

The first level of asphalt omics elucidates the relationship between the material composition and properties, forming the basis for asphalt classification, targeted modification, and innovative design. The second level addresses the interplay among design parameters, production variables, and construction practices to optimize structures and extend service life. The third level focuses on the environmental impacts of asphalt pavements, linking emissions to human health and sustainability, and promoting the use of low-emission materials and economically friendly technologies. These three levels support the development of advanced materials and sustainable roads. In summary, asphalt omics integrates material properties, structural characteristics, and environmental impacts within a data-driven, multiscale framework, leveraging high-throughput testing, big data analytics, and intelligent databases to enhance material design, construction quality, and sustainability.

3. Asphalt omics test platform

Testing platforms provide critical pathways for elucidating the functional units, internal logic, and operating mechanisms of asphalt, underpinning the analysis platforms and databases. By capturing extensive micro- and macroscale data, test platforms enable comprehensive characterization that surpasses conventional methods focused on isolated features. By integrating chemical, microstructural, and mechanical data within a high-throughput, data-centric framework, testing platforms can transform fragmented empirical observations into coherent, system-level insights, supporting data-driven modeling and sustainable pavement innovation.

3.1. Fractionation analysis

Asphalt fractionation serves as a pretreatment step in asphalt omics, improving analytical resolution by minimizing component interference and streamlining subsequent analyses. Chromatography, the primary fractionation technique, categorizes components based on molecular interactions (Fig. 3).

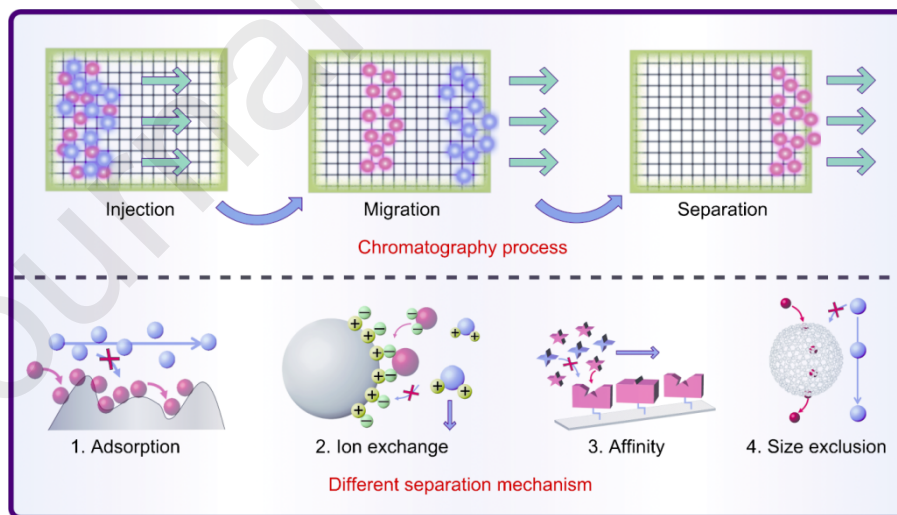


Fig. 3. Principles of chromatography for asphalt fractionation.

Theoretically, asphalt can be fractionated indefinitely to reduce component interference and simplify complex chemical profiles; however, maintaining the representativeness, independence, and functionality of each fraction remains critical. ASTM D4124-09 remains the standard method; however, its effectiveness is limited by overlapping elution and weak correlations with material properties [17]. Fractionation based on solubility, molecular weight, and

3.2. Elemental composition analysis

In asphalt material omics, elemental composition is intrinsically linked to asphalt properties. The types and contents of elements—whether inherent, introduced through modification, or formed through reactions—significantly determine performance under various conditions. The impact of various elements on asphalt, highlighting their contributions to the overall properties and their importance in the development of high-performance, functional pavement materials, is shown in Fig. 4 [18–42].



In asphalt pavement omics, elemental composition influences pavement performance. Oxygen and nitrogen improve asphalt–aggregate adhesion and tensile strength, whereas sulfur, phosphorus, calcium, and magnesium influence the wetting properties. Silicon, aluminum, and iron strengthen the asphalt–aggregate bond [43]. Elements, such as calcium, silicon, and oxygen, are critical to the interfacial transition zone, whereas carbon-based mineral additives enhance the performance and reduce hazardous leaching [44]. Specific aggregates contribute to durability (Ca), high-temperature stability (Mg), and wear resistance (Al), whereas Cu and Fe enhance the conductivity and skid resistance [45].

In asphalt environmental omics, the elemental composition also shapes environmental impact. Asphalt releases light elements and heavy metals during heating and weathering, affecting the soil and air quality. Road construction elevates the levels of polycyclic aromatic hydrocarbons (PAHs), particulate matter, and toxic elements in surrounding air [46]. Elements, such as calcium, silicon, and sulfur, help distinguish asphalt from tire particles [47], whereas transition metals such as iron, copper, and nickel catalyze the formation of free radicals under ultraviolet (UV) radiation, accelerating material aging. Although external elements, such as Ti and Zn, can function as antioxidants, their potential to cause secondary pollution must be considered.

Developing a comprehensive elemental database will expedite the design of novel pavement materials, inform construction practices, and support environmental impact assessments. Although asphalt comprises a limited range of elements, their interactions are complex, involving bonding mechanisms, electron transfer, hydrogen bonding, and van der Waals forces. Multi-level analyses are essential to quantify elemental content and functional groups in asphalt, and to understand the influence of their combinations on performance [48]. External factors, such as thermal oxidation, UV radiation, and pH variations, significantly alter the elemental composition of asphalt, and should be systematically investigated [49].

3.3. Molecular interactions analysis

Molecular interactions analysis in asphalt research centers on identifying the chemical bonds and functional groups that govern material reactivity. Spectroscopic techniques provide detailed molecular insights into complex structures, elucidating the impacts of various bonding environments and functional groups on asphalt properties (Fig. S2 in Appendix A). These methods also reveal molecular dynamics (MD), intermolecular interactions, and variations, deepening our understanding of the underlying mechanisms of asphalt.

(1) Infrared (IR) spectroscopy and ultraviolet–visible (UV–Vis) spectroscopy. IR spectroscopy is a critical tool for analyzing the functional groups and chemical bonds within asphalt, encompassing near-infrared (NIR), mid-infrared (MIR), and far-infrared (FIR). NIR detects overtones and combination bands from lighter atoms, such as C–H and O–H, whereas FIR relates to molecular rotations and vibrations [50]. MIR provides the most detailed structural information, covering both the characteristic (4000–1500 cm^{-1}) and fingerprint (1500–400 cm^{-1}) regions. The fingerprint region captures unique vibrational patterns, enabling precise molecular identification. However, overlapping absorption bands can complicate spectra interpretation. To address this, advanced techniques, such as two-dimensional correlation spectroscopy and ML algorithms, have been employed to enhance spectral analysis. Changes in functional groups revealed the reaction mechanisms and performance of the asphalt under different conditions. External factors and modifiers alter the chemical bonds and functional groups of asphalt, thereby regulating its performance. The insights from the functional group variations are listed in Table S3 in Appendix A.

UV–Vis spectroscopy is widely utilized to evaluate the UV absorption and aging resistance of asphalt materials

[51]. By detecting electronic transitions, UV-Vis provides complementary information on aromatic rings, heterocyclic compounds, and other light components, supporting IR analysis. UV-vis spectroscopy can refine the absorption profiles of aromatic fractions [52], differentiate asphalt types based on solution absorbance, and detect VOCs within the UV range [53]. However, UV-Vis is limited to chromophore-containing compounds and cannot effectively characterize non-conjugated aliphatic structures, restricting its broader application.

Integrating ML algorithms with spectroscopic analysis has significantly enhanced spectral data interpretation by identifying key features and capturing nonlinear relationships with asphalt performance metrics. For example, saturates, aromatics, resins, and asphaltenes (SARA) fraction models based on UV-vis spectra [54] and rheological parameter prediction models using IR data [55] demonstrated this potential. Support vector machines deliver superior predictive performance for asphalt viscoelastic properties compared with other ML algorithms [56]. Additionally, the concept of “asphalt genes,” which utilizes IR spectra to define structural units associated with asphalt properties, presents a transformative approach to asphalt characterization [57]. Overall, data-driven spectral analysis enhances predictive accuracy and deepens understanding of the mechanisms underlying asphalt behavior.

(2) Nuclear magnetic resonance (NMR). NMR provides detailed insights into the molecular structure and chemical environment of asphalt, revealing atomic connectivity, functional group distribution, and MD. ^{13}C -NMR distinguishes carbon types in aromatic rings, aliphatic chains, and heterocycles, whereas ^1H -NMR characterizes hydrogen atoms within these frameworks. Each atom and functional group produced unique chemical shifts, reflecting their specific environments. Additionally, relaxation times provide further details on MD, making NMR a versatile tool for probing asphalt structures. The commonly used NMR parameters are listed in Table S4 in Appendix A.

In asphalt omics, NMR is crucial for directly linking molecular composition and performance. ^{13}C -NMR has been employed to trace asphalt origins and elucidate structural differences, thereby providing insights into the diversity of the source materials [58]. Variations in hydrogen content identified through ^1H -NMR highlight the chemical complexity of different asphalts, and chemical shifts can differentiate asphalt types [59]. NMR is closely linked to material properties; for example, crystallized methylene carbon content correlate with wax levels, demonstrating its prediction potential.

NMR is essential in developing modified asphalt databases, as additives produce distinct signal shifts that reflect compositional and property changes [60]. The relationship between aromatic ring content and low-temperature performance further demonstrates the value of NMR in performance evaluation. ML has been employed to connect NMR data with rheological properties, enhancing prediction accuracy [61]. Converting NMR spectra into numerical matrices enables the differentiation of samples based on aging, additives, and molecular structure. Integrating NMR with techniques, such as IR spectroscopy, supports multiparameter models for viscosity, enhancing analytical efficiency and understanding molecular interactions [62].

NMR has been increasingly applied to asphalt mixtures and pavements. The relative hydrogen index from low-field NMR correlates closely with the mixture performance [63], whereas relaxation rates are associated with pore structure parameters [64]. Portable NMR devices facilitate rapid, non-destructive, on-site assessments of pavement conditions, including moisture damage and porosity. Furthermore, NMR has been employed in non-destructive testing of rubber distribution [65], and primary relaxation times. Their ratios help determine the asphalt performance grade [66]. By analyzing hydrogen proton relaxation times in pore fluids, NMR can evaluate the porosity and provide indirect information on pore size distribution and volume, rendering it well-suited for saturated systems [67]. These advancements highlight the critical role of NMR in linking molecular structure to engineering performance.

(3) Mass spectrometry (MS). MS determines the molecular mass and structure by ionizing samples and measuring the mass-to-charge ratio (m/z) of ions, enabling precise quantification and identification of complex asphalt components.

MS-based approaches have significantly advanced asphalt database development by enabling the quantitative analysis of chemical structures, differentiation of asphalt types, and correlation of specific asphalt compounds with physical properties. Moreover, MS reveals chemical reactions and modification mechanisms [68], providing insights into molecular changes during chemical modification, thermo-oxidative aging, and pyrolysis [69].

Furthermore, MS evaluates environmental impacts by detecting asphalt components in air, water, and soil. MS has been utilized to identify VOCs emitted during construction, develop VOC emission models, and investigate pollutants relevant to human exposure. MS detects pollutants in runoff and soil, elucidating the impact of additives on water quality [70]. Furthermore, medical MS analyzes biological samples to identify asphalt-related compounds and metabolites, linking road materials to human health. Compared with other methods, MS provides more comprehensive support for health and environmental evaluations.

Recent advancements in spectroscopy have further enhanced asphalt characterization. As shown in Fig. 5 [71–74], techniques, such as spectrum stitching (Fig. 5(a) [71]), correlation (Fig. 5(b) [72]), and differencing (Fig. 5(c) [73]), have expanded the scope of MS in asphalt research. Spectral imaging (Fig. 5(d) [74]) integrates spectroscopy with imaging to provide spatial and chemical composition data microscopically, thereby offering a more comprehensive understanding of asphalt microstructures.

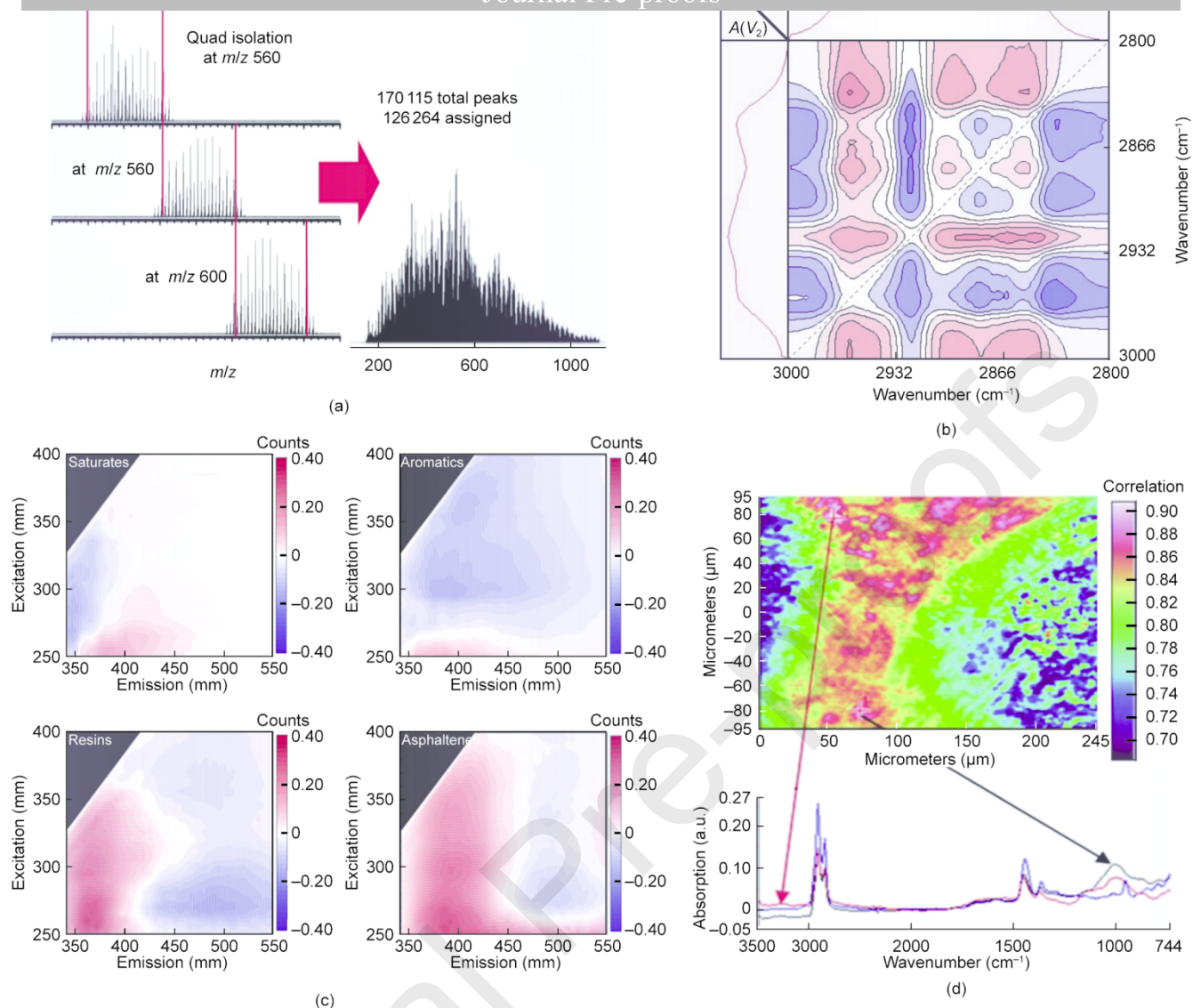


Fig. 5. Advanced spectrum analytical techniques for mass spectrometry. (a) Spectrum stitching. Reproduced from Ref. [71] with permission. (b) Spectrum correlating. Reproduced from Ref. [72] with permission. $A(V_1)$ and $A(V_2)$ denote the dynamic absorbance spectra corresponding to V_1 and V_2 , respectively, where V represents the external perturbation parameter. (c) Spectrum differencing. Reproduced from Ref. [73] with permission. (d) Spectrum imaging. Reproduced from Ref. [74] with permission.

In asphalt omics, IR spectroscopy identifies primary functional groups, UV–Vis spectroscopy provides information on conjugated systems, NMR provides chemical environment data, and MS offers a detailed molecular structural analysis. Integrating conventional and advanced spectroscopic techniques is essential for developing comprehensive asphalt spectral databases and enhancing material characterization and performance prediction.

However, conventional spectroscopic techniques have limitations at the omics level. Fourier-transform infrared spectroscopy (FTIR) often experiences band overlap and limited resolution for trace components, whereas UV–Vis spectroscopy is primarily sensitive to conjugated systems and cannot detect non-chromophore aliphatic compounds. NMR requires high sample purity and solubility, restricting its application to high-viscosity, complex asphalt samples. MS, despite its sensitivity, involves complex preparations and can cause molecular fragmentation, which complicates data interpretation. To address these challenges, advanced techniques have been developed. Two-dimensional

correlation spectroscopy enhances resolution and captures molecular interactions, whereas solid-state NMR enables analysis of rigid, insoluble samples. Fourier transform ion cyclotron resonance (FT-ICR) MS provides unrivaled mass resolution for complex mixtures. Nondestructive methods, such as Raman spectroscopy and X-ray absorption spectroscopy, provide detailed insights without extensive sample preparation. Hyphenated techniques, including comprehensive two-dimensional gas chromatography–MS and liquid chromatography–NMR, integrate separation and detection to minimize spectral overlap. These methods strengthen asphalt omics platforms, enabling more precise material characterization and performance prediction.

3.4. Molecular structure analysis

Molecular structure analysis is essential in asphalt science, as the macroscopic properties of asphalt depend not only on elemental composition and chemical bonds but also on the spatial arrangement and interactions of its molecular structures. This analysis identifies representative molecular configurations that govern performance and provides a foundation for understanding the influence of molecular architecture on material behavior.

(1) **Molecular structure and simulation of asphalt.** The concept of average molecular structure was first introduced by Brown et al. [75], whose early models captured the molecular differences among asphalt types and laid the foundation for analyzing organic petroleum products. Subsequent research refined these models and extended their application to aged asphalt [76], recycled asphalt, and various grades and sources. Examples are shown in Fig. S3 in Appendix A.

However, asphalts with similar average molecular structures demonstrate significant performance variations. Developing average structures for each SARA fraction helps elucidate on these differences [77]. This approach supports the development of asphalt omics databases by enabling the selection of fractions with diverse proportions and structures [78]. Common models include 4-, 12-, and 16-component systems [79]. Wax and asphaltene structures have received particular attention [80], and the methodology has recently been applied to modified asphalts to investigate the impact of modifiers [81].

With advances in the understanding of asphalt molecular structure, asphalt omics seeks to create a comprehensive molecular atlas that captures the complexity of asphalt composition. Petroleomics, with over two decades of experience, has established digital databases cataloging the chemical diversity of petroleum, providing a valuable reference for the development of asphaltomics [82]. The petroleomic data analysis and potential pathways for advancing asphaltomics are shown in Fig. 6 [83–86], including data mapping (Fig. 6(a) [83]), Ag⁺-complexation electrospray ionization high-resolution mass spectrometry (ESI-HRMS) (Fig. 6(b) [84]), double bond equivalent (DBE)-carbon-number classification (Fig. 6(c) [85]), and drift time–m/z ion-mobility separation (Fig. 6(d) [86]). Collectively, these approaches provide methodological references for advancing asphalt omics. Petroleomics integrates chemical analysis, colloid chemistry, and cheminformatics, providing tools for elucidating structure–function relationships in complex hydrocarbon systems. For example, research has demonstrated its role in uncovering crude oil and asphaltene complexities [87] and in demonstrating advanced analytical techniques applicable to asphaltomics [88].

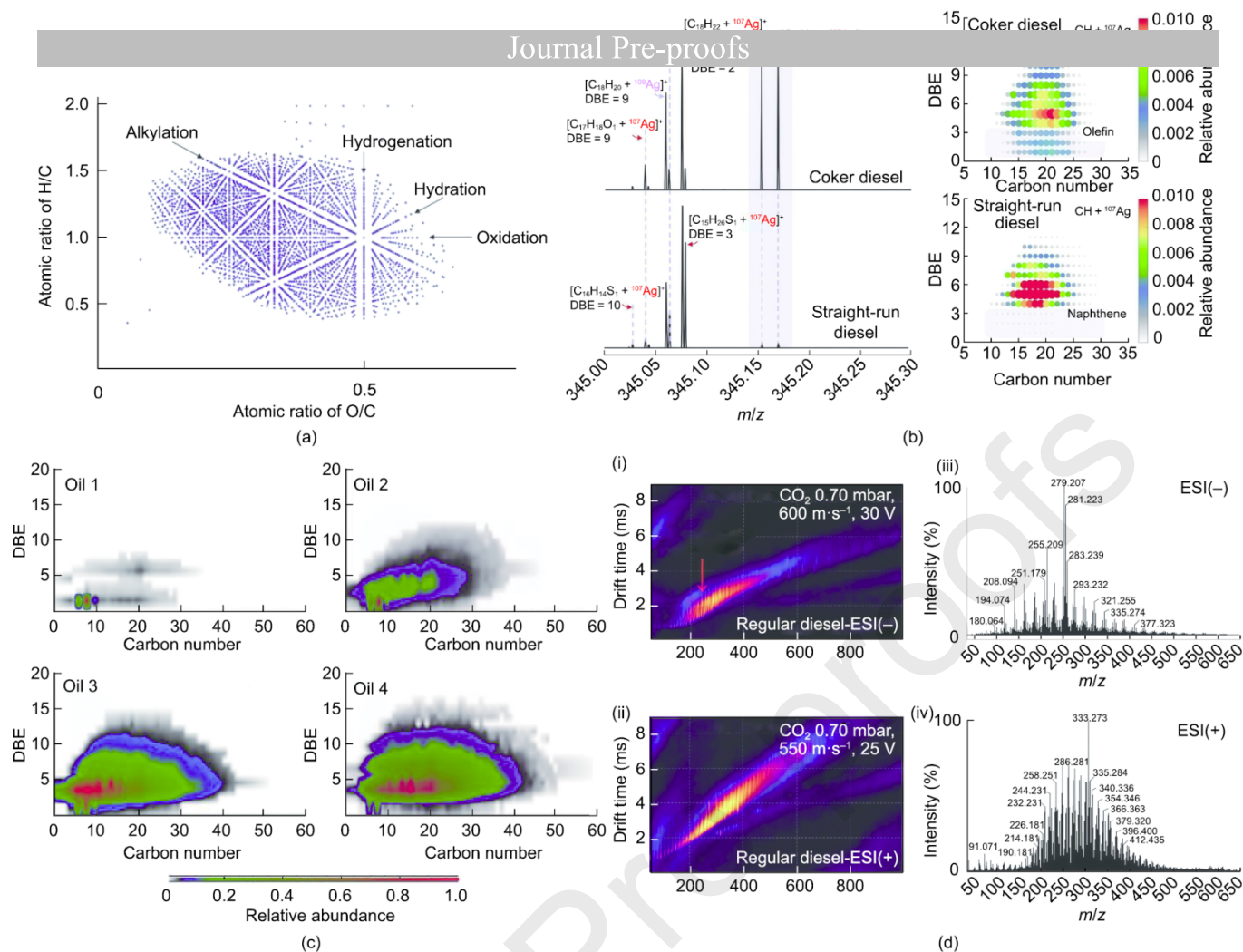


Fig. 6. Omics data analysis techniques. (a) van Krevelen plot (ultrahigh-resolution mass spectrometry (URMS) data). Reproduced from Ref. [83] with permission. (b) Ag⁺ complexation and ESI-HRMS analysis. Reproduced from Ref. [84] with permission. (c) DBE versus carbon number (O₂ class, four crude oils). Reproduced from Ref. [85] with permission. (d) Two-dimensional drift time versus m/z plot (ESI(-) and ESI(+)). Reproduced from Ref. [86] with permission. H/C represents hydrogen-to-carbon atomic ratio; O/C represents oxygen-to-carbon atomic ratio.

MD simulations have enhanced molecular-level investigations of asphalt; however, their application in large-scale or long-timescale systems is limited by significant computational demands. Additionally, the accuracy of MD is constrained by force fields that lack comprehensive parameterization for asphalt, resulting in oversimplified representations of intermolecular interactions and mechanical properties. MD typically assumes homogeneity, overlooking molecular heterogeneity and environmental variability, potentially leading to discrepancies with experimental results. Integrating MD with quantum chemical methods, such as density functional theory and AI techniques, holds promise for improving both the accuracy and efficiency of molecular behavior prediction.

Quantum chemical methods model the electronic environments of atoms and functional groups, capturing bond formation, dissociation, and electron density distributions that govern molecular stability and reactivity. These methods enable atomic-scale simulations of reaction pathways and intermolecular interactions, providing as a valuable complement to conventional approaches for high-resolution asphalt genomics modeling. Integration with AI further enhances predictive capabilities. ML frameworks now support real-time predictions of molecular systems and facilitate modeling of structure-activity relationships in asphalt molecules [89]. High-throughput MD platforms generate models with varying SARA ratios and aging levels, improving simulation precision through extensive training datasets. Real-time feedback systems using atomic-type inputs allow for instant chemical feature prediction. Deep learning (DL) has

also been applied to autonomously construct time-dependent optimal control fields in dynamic systems. Combined with high-throughput experimental data, these approaches address conventional limitations of MD, enhance predictive accuracy, and deepen the understanding of asphalt behavior.

(2) **Molecular structure and asphalt omics.** Understanding the molecular structure of asphalt is crucial for understanding the microstructure–performance relationship and enabling molecular-level material design. In asphalt omics, comprehensive molecular databases and advanced data analysis methods are essential for elucidating composition–performance relationships. Classic behaviors, such as self-healing, phase transitions, and aging, have been characterized at the molecular level. The effects of modifiers and rejuvenators were also explored, informing strategies for asphalt optimization and recycling. Molecular design has enabled the precise engineering of functional additives.

Environmental factors significantly influence the molecular structure and performance of asphalts. UV radiation and reactive oxygen species can alter the molecular structures, changing rheological and mechanical properties. MD simulations elucidated these long-term molecular changes, whereas molecular studies have advanced understanding of rejuvenator diffusion and binder blending during recycling. Such research also facilitates evaluation of asphalt–environment interactions, including VOC emissions and leaching of harmful elements—critical for assessing impact on human health and ecosystems [90]. Notably, the United States Environmental Protection Agency has designated 16 PAHs as high-priority pollutants [91].

The key objective of asphalt omics is the controlled design of materials that optimize performance, cost, and environmental sustainability through precise molecular control. Molecular design has been widely applied to both chemical and asphalt materials. Representative case studies, such as recyclable epoxy asphalts that enhance recyclability and reduce carbon footprint, are shown in Fig. S4 in Appendix A [92]. Molecular weight-based design strategies have enhanced the compatibility of highly viscous modified asphalts [93]. ML and MD have further refined asphalt formulations for tailored performance. Furthermore, molecular design has yielded novel resin additives to boost durability and enabled the direct prediction of modifier effects, minimizing the need for experimental validation.

Molecular design provided a robust approach for developing asphalt materials by enabling precise control of molecular structures to optimize the performance and satisfy functional requirements. Unlike empirical approaches, this method allows for the targeted adjustment of molecular parameters that determine performance, supports high-throughput exploration of compositional variations, and accelerates product development with the desired characteristics. Molecular design is particularly valuable for engineering functionalized and environmentally friendly materials, as well as for designing additives that align with asphalt omics trends. With advancements in these technologies, molecular design is expected to drive more cost-effective, sustainable materials, and tailored solutions for engineering applications.

3.5. Microstructure analysis

Asphalt properties are determined by its chemical composition and microstructure, which reflects the arrangement, crosslinking, and aggregation of molecular components [94]. These features govern the mechanical strength, durability, and rheological behavior. Unlike purely chemical characteristics, the microstructure of asphalt is influenced by its stress history and environmental exposure, resulting in heterogeneity and structural complexity. Adopting a microstructural perspective enables a more comprehensive understanding of asphalt behavior and its impact on performance.

Advanced imaging techniques, such as optical microscopy, transmission electron microscopy (TEM), scanning electron microscopy (SEM), atomic force microscopy (AFM), and scanning tunneling microscopy (STM), provide critical insights into asphalt microstructure, as shown in Fig. 7. These methods reveal details ranging from nanoscale interactions to surface morphology and aggregate distribution. Information commonly utilized in microstructural studies is listed in Table S6 in Appendix A.

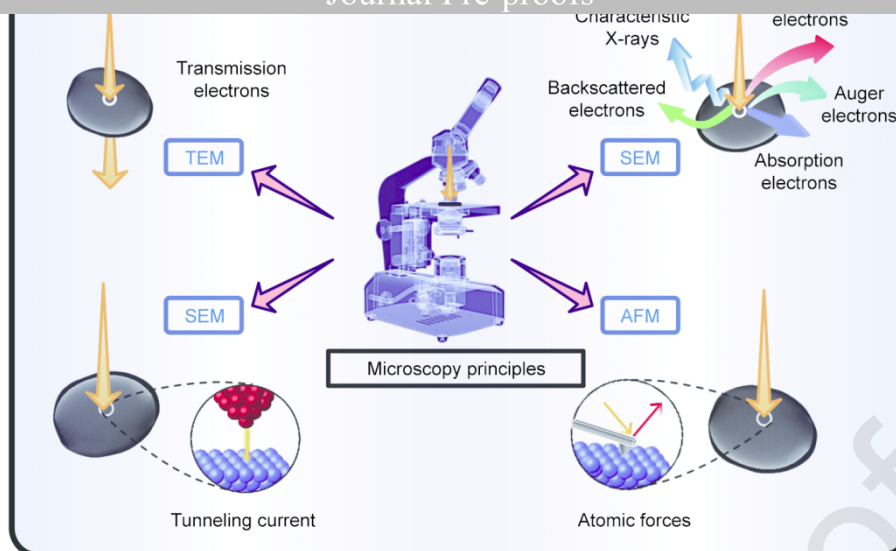


Fig. 7. Principles of microscopy techniques in asphalt characterization.

Microstructural differences help differentiate asphalt types. Asphaltene content influences the structure, size, and shape of bees [95], whereas crystalline wax influences their formation [96,97]. Wax-free asphalts demonstrate smoother surfaces, whereas asphaltene-rich asphalts display more pronounced microstructures [98]. Integrating chemical analysis with microstructural observations yields a comprehensive understanding of asphalt bee structures that correlate with asphaltene content, metals, and linear n-alkanes. The physical states of wax and asphaltenes significantly impact performance: Asphaltenes form aggregates that increase viscosity. In contrast, crystalline wax promotes phase separation and reduces flexibility. Microstructural features, such as bee structures and the island-to-archipelago ratio observed in AFM images, can be employed to identify asphalt types, processing histories, and predict performance [99,100].

Understanding microstructural evolution is essential for predicting asphalt performance and characterizing processes, such as modification, aging, and rejuvenation [101]. For example, aging increases nanoscale roughness [102], whereas rejuvenators can cause spatial adjustments without fully restoring the original microstructure [103]. A major challenge in developing a micromorphology-based asphalt database is selecting parameters with sufficient discriminatory power to predict the performance. Effective parameters should capture critical structures and correlate with key indicators, enabling automated, data-driven characterization. The relationships between the AFM parameters and viscoelastic or fatigue properties are well documented, with established correlations between AFM images, SARA fractions, and mechanical properties. Bee structures are widely used to evaluate the aging resistance [104]. Quantifiable parameters for the polymer-modified asphalt morphology, as well as the link between styrene-butadiene-styrene (SBS) molecular structure and microstructure, have been investigated. Representative microstructure images collected over the past decade are shown in Fig. 8 [98,105–120]. However, standardizing and integrating these parameters across diverse imaging technologies remains a challenge as new analytical tools continue to emerge.

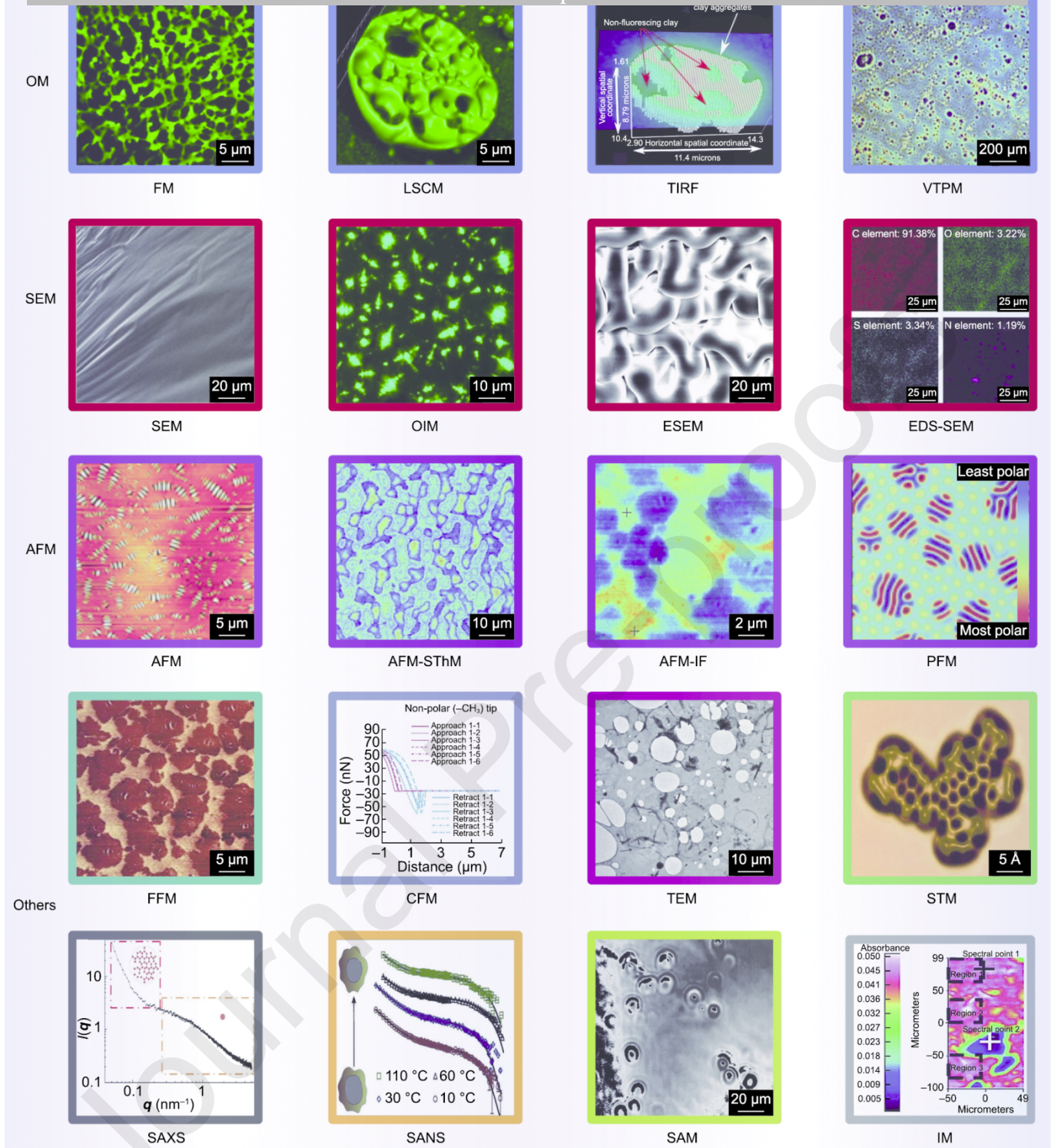


Fig. 8. Microscopic characteristics of asphalt under different microscopic techniques: fluorescence microscopy (FM) [105]; laser scanning confocal microscopy (LSCM) [106]; total internal reflection fluorescence (TIRF) microscopy [107]; video-rate time-resolved polarized microscopy (VTPM) [108]; SEM [109]; optical interference microscopy (OIM) [110]; environmental scanning electron microscopy (ESEM) [111]; energy-dispersive spectroscopy coupled with SEM (EDS-SEM) [112]; TEM [113]; AFM [98]; AFM–scanning thermal microscopy (AFM–SThM) [114]; AFM–intermodulation force microscopy (AFM–IF) [114]; friction force microscopy (FFM) [114]; chemical force microscopy (CFM); piezo response force microscopy (PFM) [115]; STM [116]; scanning acoustic microscopy (SAM) [117]; small-angle X-ray scattering (SAXS) [118]; small-angle neutron scattering (SANS) [119]; and interferometric microscopy (IM) [120]. Reproduced from Refs. [105–120] with permission. q : scattering vector; $I(q)$: scattering intensity.

The microscopy techniques shown in Fig. 8 [98–105, 120] include fluorescence microscopy (FM), laser scanning confocal microscopy (LSCM), total internal reflection fluorescence (TIRF) microscopy, video-rate time-resolved polarized microscopy (VTPM), optical interference microscopy (OIM), environmental scanning electron microscopy (ESEM), energy-dispersive spectroscopy coupled with SEM (EDS-SEM), AFM–scanning thermal microscopy (AFM–SThM), AFM–intermodulation force microscopy (AFM–IF), friction force microscopy (FFM), chemical force microscopy (CFM), piezo response force microscopy (PFM), scanning acoustic microscopy (SAM), small-angle X-ray scattering (SAXS), small-angle neutron scattering (SANS), and interferometric microscopy (IM).

A systematic approach is required to standardize the microstructural parameters across these techniques. Parameters must first be clearly defined and correlated with key asphalt properties, including surface roughness, phase distribution, and aggregate morphology. Consistent standards for sample preparation, image resolution, and pixel density are essential to ensure comparability. Once established, interrelationships among parameters can be explored. Finally, advanced image recognition can automate parameter extraction, whereas data-driven models can leverage standardized descriptors to predict performance.

Although the omics paradigm has significantly advanced biological sciences, its application to asphalt, a non-living, chemically diverse, and structurally complex material, presents unique challenges. Conventional omics techniques focus on well-defined biomacromolecules, whereas asphalt comprises undefined molecular populations with wide-ranging molecular weights, functionalities, and aggregation states. This complexity hinders the identification of clear analytical targets and the establishment of typical pathways, as asphalt lacks the hierarchical networks observed in biological systems. External factors, such as temperature, oxidation, and mechanical stress, serve as environmental perturbations rather than eliciting programmed responses. Addressing these challenges requires advanced tools to define asphalt-specific functional units, such as structural motifs or supramolecular domains. Therefore, developing cross-dimensional frameworks that integrate compositional, morphological, and mechanical features is essential. Data-driven modeling and ML can facilitate the construction of transformation pathways and the identification of key environmental drivers, even when asphalt changes are irreversible. Advances in asphalt omics will depend on enhanced testing capabilities and integration of intelligent analyses and data platforms. Only through this synergy can the omics paradigm deepen our understanding of asphalt composition–structure–property relationships and drive innovation in materials and pavement engineering.

4. Asphalt omics analysis platform

4.1. Artificial intelligence in asphalt omics

As data on asphalt omics platforms become increasingly complex and multidimensional, conventional analytical methods are no longer adequate. To address these challenges, advanced platforms must incorporate cutting-edge analysis technologies, with AI at the core. Knowledge graphs (KG) integrate data across multiple layers, providing structured maps that reveal dynamic relationships between sources [121]. Natural language processing (NLP) extracts and summarizes key insights from unstructured text [122]. Multi-agent systems (MASs) enable communication and collaboration among devices, thereby improving industrial efficiency [123]. ML enhances the accuracy and efficiency of data processing, whereas computer vision (CV) automates image analysis for improved data representation and interpretation [124]. The integration of multiple AI technologies enhances data interpretation, intelligent decision-making, and system integration in asphalt omics platforms.

AI is revolutionizing materials science by enabling the discovery of novel chemical structures, accelerating simulations, and enhancing property predictions. As shown in Fig. 9 [125–128], applications include reverse molecular design (Fig. 9(a) [125]), unsupervised microstructure characterization (Fig. 9(b) [126]), AI-enabled design and management in Building and Construction 4.0 (Fig. 9(c) [127]), and data-driven polymer screening and optimization (Fig. 9(d) [128]), offering methodological insights relevant to advancing asphalt omics. Advanced models, such as

message-passing neural networks are effective for complex molecular modeling beyond conventional methods. In polymer science, AI has enhanced viscosity predictions through thermodynamic modeling and facilitated advanced polymer designs using data-driven frameworks [129]. Similarly, ML and DL demonstrate significant potential for predicting material performance, including mechanical properties and durability [130].

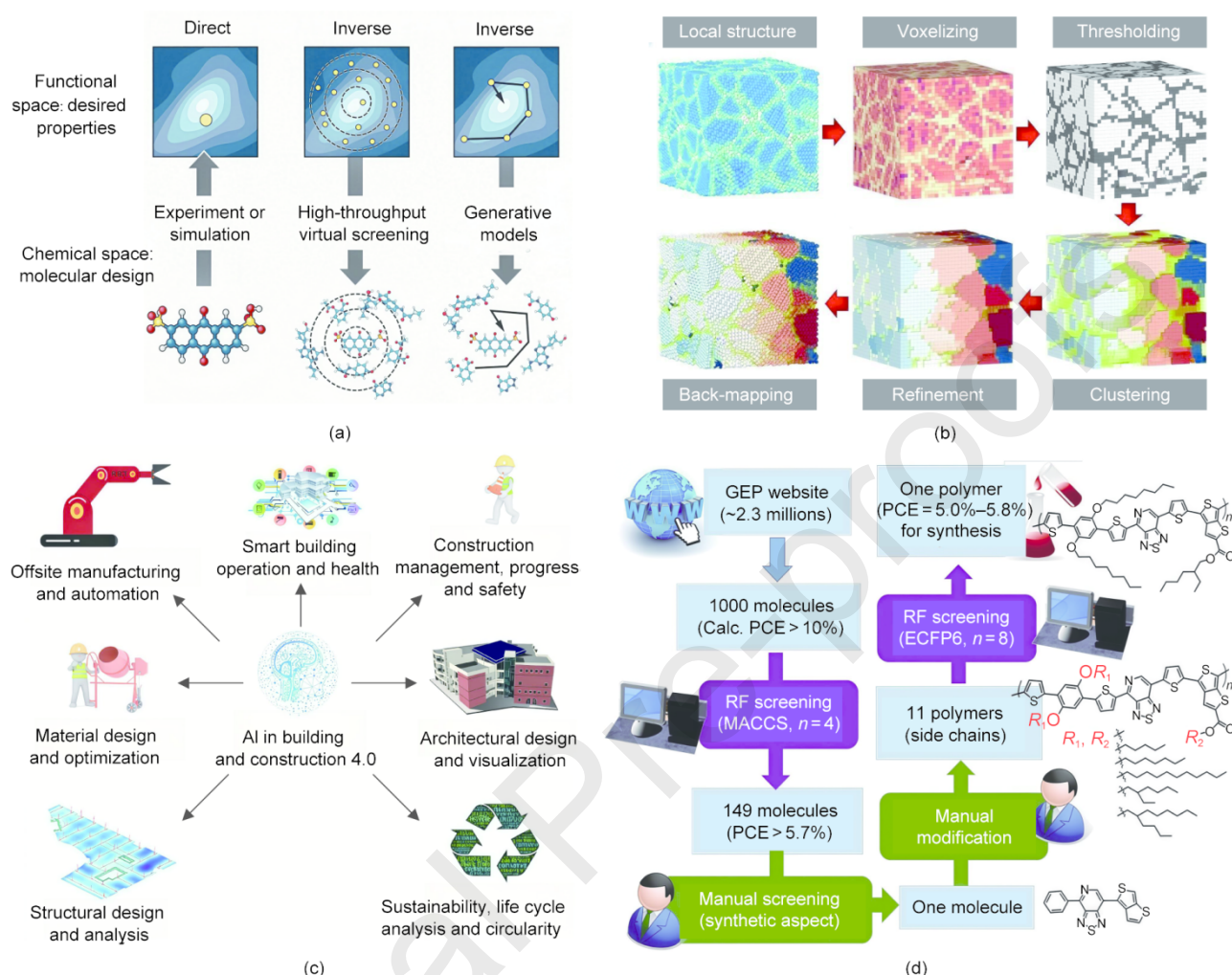


Fig. 9. Applications of AI in materials science and engineering. (a) Reverse molecular design through ML. Reproduced from Ref. [125] with permission. (b) Unsupervised three-dimensional (3D) microstructure characterization. Reproduced from Ref. [126] with permission. (c) AI in Building and Construction 4.0. Reproduced from Ref. [127] with permission. (d) Polymer design with ML and manual screening. Reproduced from Ref. [128] with permission. CEP: clean energy project database; Calc. PCE: calculated power conversion efficiency; ECFP6: extended connectivity fingerprint with diameter 6; MACCS: molecular access system; PCE: power conversion efficiency; R_1 and R_2 : variable substituent groups (side chains); RF: random forest; n denotes the number of PCE classification groups used in the RF model.

4.2. Machine learning in asphalt omics

The effectiveness of AI significantly depends on its underlying algorithms, which are essential for data processing, model training, and decision-making. Key AI techniques, including supervised, unsupervised, semi-supervised, and reinforcement learning, are each suited to specific tasks and datasets. The logical principles of these learning types and a comparative overview are shown in Fig. 10.

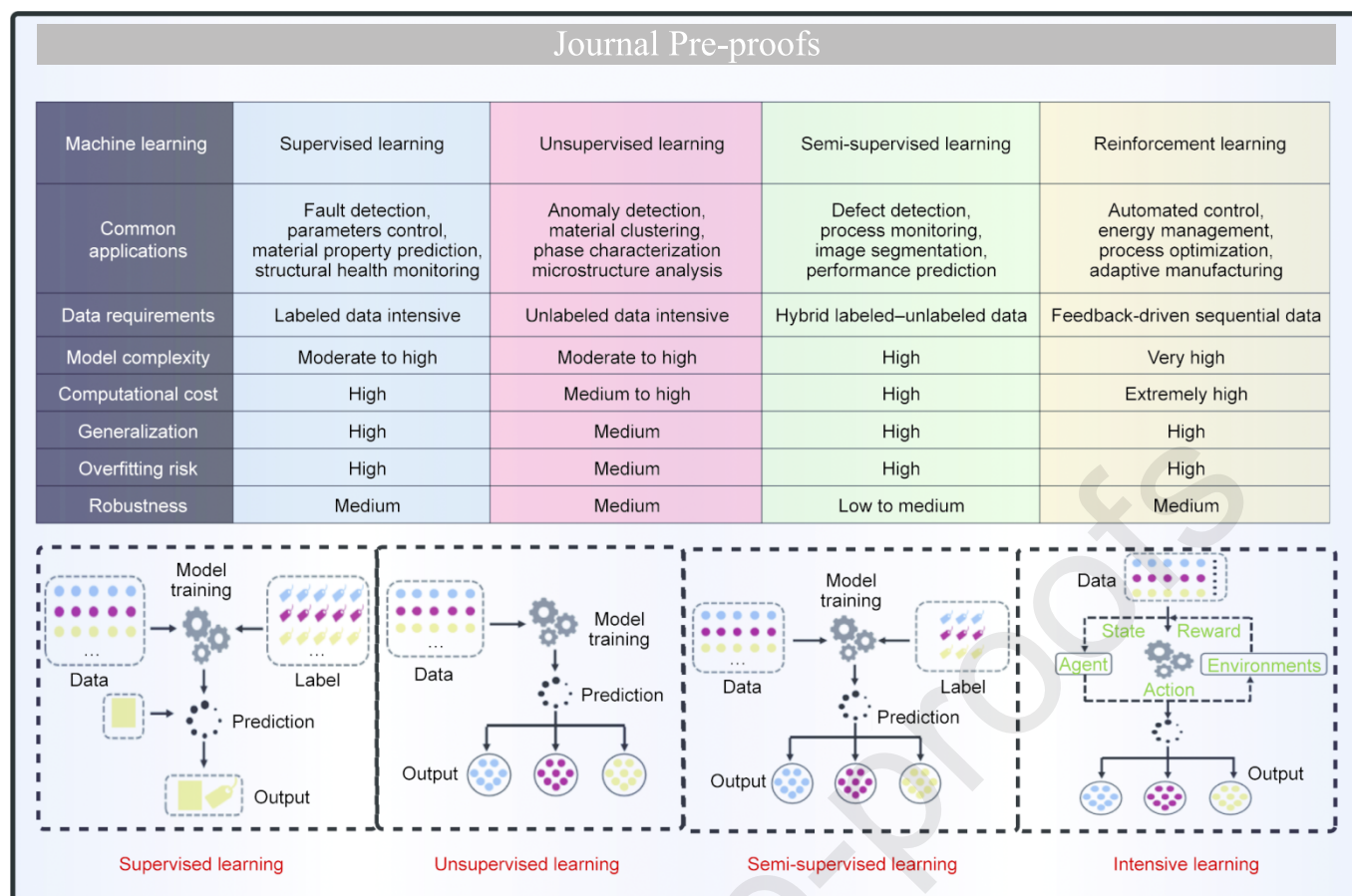


Fig. 10. Typical algorithms for different categories of ML applications.

In asphalt omics, ML paradigms address various data types and tasks. Supervised learning leverages labeled data to predict asphalt properties from micro-level features and performance indicators [131]. Unsupervised learning identifies hidden patterns in unlabeled data, enabling clustering and dimensionality reduction to identify compositional variability. Semi-supervised learning combines labeled and unlabeled data to improve generalization and uncover associations when only a subset of samples has known metrics [132]. Reinforcement learning optimizes multi-objective material designs by iteratively refining formulations based on simulated feedback to balance performance and cost.

In addition to material design, ML also advances pavement and environmental omics. Supervised learning facilitates pavement structure optimization, construction quality control, and maintenance planning. Unsupervised learning uncovers patterns in working conditions and assesses the impact of environmental factors on pavement durability [133]. Semi-supervised learning integrates multi-source sensing data with limited labels to enhance long-term predictions and condition recognition [134]. Reinforcement learning enables adaptive, feedback-driven processes for intelligent construction and maintenance. Integrating these paradigms supports intelligent decision-making across the asphalt lifecycle—from material development to pavement management and environmental evaluation—accelerating sustainable, data-driven infrastructure.

ML adoption in asphalt research has increased, transforming the prediction and optimization of binder properties, pavement quality, and environmental impacts. Advances in computational power and data processing have enabled the efficient analysis of large-scale asphaltomics datasets, driving insights and innovations in material design. Representative applications of ML in asphalt science, including binder rutting parameter prediction [135], asphalt mixture design optimization [136], estimation of asphalt layer elasticity modulus [137], and VOC-related risky substance identification [138] are shown in Fig. S5 in Appendix A, encompassing characterization, structural design, performance prediction, and environmental monitoring.

In asphalt material omics, ML models are essential for predicting binder properties, including rheological, mechanical, and durability characteristics [139]. These models forecast specific attributes, such as stiffness, elasticity, and aging resistance, and help identify optimal analytical strategies to enhance material performance. Numerous studies provide guidance on algorithm selection, data preprocessing, and feature engineering to improve prediction accuracy. A range of these applications, outlining the specific targets addressed, algorithms employed, and recommended approaches for optimizing asphalt binder performance, is listed in Table S7 in Appendix A.

In asphalt pavement omics, ML-driven methods significantly enhance the prediction of mechanical performance, optimization of mixture designs, and reduction of design costs. These approaches address a broad spectrum of performance metrics, including load-bearing capacity, fatigue resistance, and long-term durability, while providing practical guidance on selecting appropriate construction parameters and maintenance strategies to enhance pavement performance. Some studies integrate sensory data for real-time pavement monitoring, whereas others highlight the value of multi-source data fusion for more accurate predictions. Table S8 in Appendix A details ML applications in asphalt mixtures, specifying performance targets, recommended algorithms, and practical strategies for optimizing mixture composition. Table S9 in Appendix A expands this focus to pavement-level applications, providing insights into structural performance optimization, real-time condition assessment, and proactive maintenance planning.

In asphalt environmental omics, ML techniques efficiently process complex datasets to evaluate the environmental impacts of asphalt materials and pavements, including their carbon footprints, resource efficiencies, and overall sustainability. These approaches facilitate the development of environmentally friendly formulations and designs by targeting emission reduction, resource conservation, and enhanced recyclability. Some studies employ ML to optimize asphalt compositions for lower emissions during production and application, whereas others focus on designing pavements with improved durability and reduced maintenance requirements, thereby extending service life and reducing environmental impact. Additionally, ML models can identify key environmental performance indicators, integrate multi-source environmental monitoring data, and generate actionable recommendations to minimize the ecological footprint of asphalt infrastructure, thereby supporting the transition to more sustainable, data-driven road systems.

4.3. Computer vision in asphalt omics

CV, a core component of AI, enables automated analysis of images and videos to extract features for decision-making. Whereas ML predicts and optimizes asphalt performance using data patterns, CV provides image-based insights into asphalt microstructure and quality. CV facilitates detailed analysis of micro- and meso-structures in asphalt binders and mixtures, as well as macro-pavement assessments. The CV applications in asphalt research are shown in Fig. 11 [140–144], including asphalt nanostructure reconstruction (Fig. 11(a) [140]), mixture microstructure image analysis (Fig. 11(b) [141]), detection and location of pavement damage (Fig. 11(c) [142]), and asphalt pavement environmental impact evaluation (Fig. 11(d) [143,144]). The number of studies in this field increases continually.

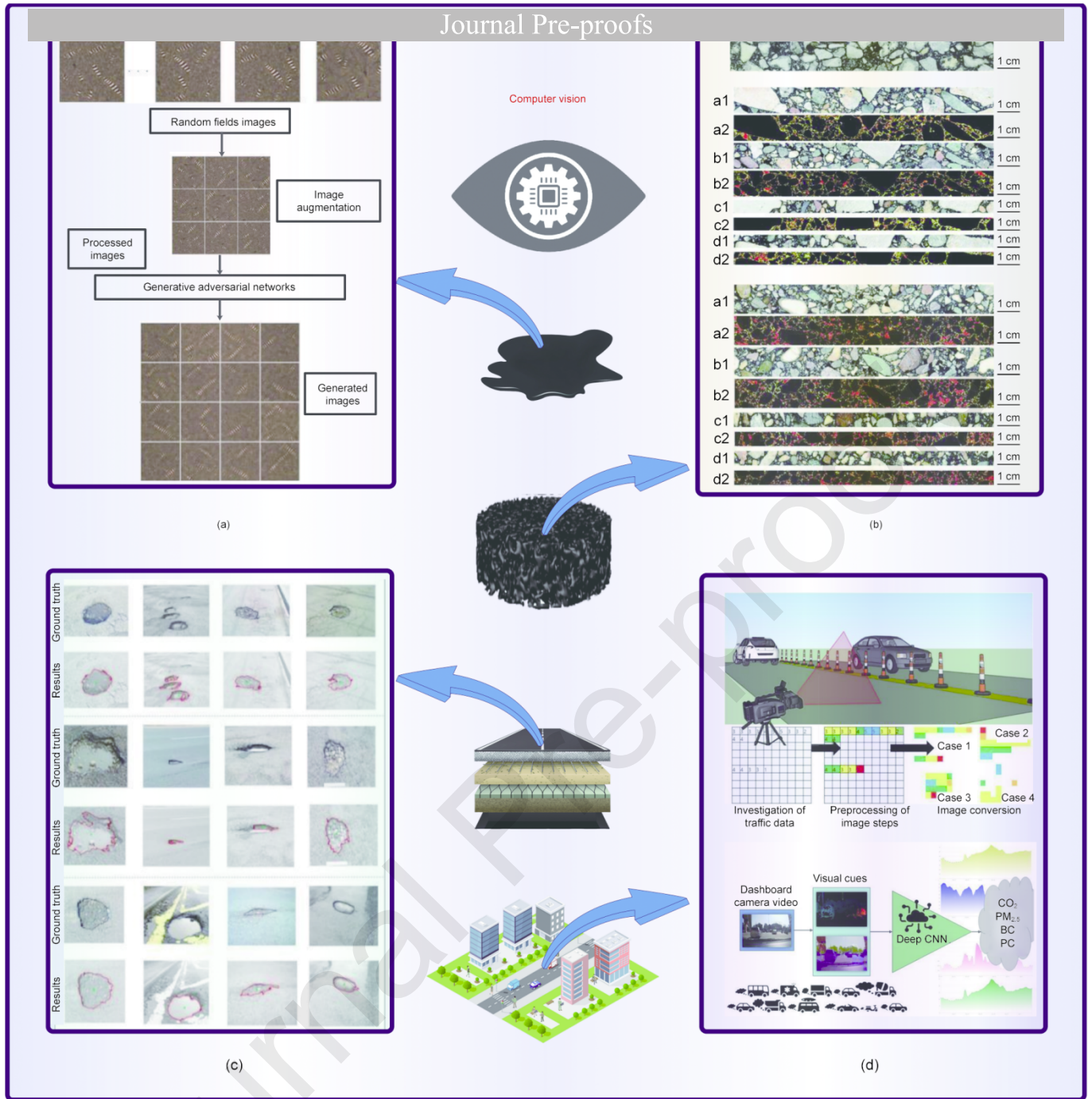


Fig. 11. Representative applications of CV in asphalt science. (a) Asphalt nanostructure reconstruction. Reproduced from Ref. [140] with permission. (b) Asphalt mixture microstructure image analysis, where a₁–d₁ are original red, green, and blue (RGB) images (top, bottom, left, and right, respectively), and a₂–d₂ are the corresponding three-phase images obtained by digital image processing. Reproduced from Ref. [141] with permission. (c) Damage to pavement detection and localization. Reproduced from Ref. [142] with permission. (d) Environmental impact assessment of asphalt pavement. Reproduced from Refs. [143,144] with permission. CNN: convolutional neural network; BC: black carbon; PC: particle concentration. PM_{2.5} represents fine particulate matter, and CO₂ is carbon dioxide.

Advancements in high-resolution imaging, deep learning, and data processing have established CV as a powerful tool for extracting critical features from asphalt materials and pavement images. CV supports characterization, inspection, monitoring, and long-term performance evaluation. By capturing and analyzing microstructural details, surface textures, and defect patterns, CV enables precise, automated assessments that were previously labor-intensive and subjective, creating a comprehensive visual evaluation system based on quantification of material properties, precise

process control, early defect detection, and continuous monitoring of pavement conditions. Various CV applications in asphalt research are listed in Table S10 in Appendix A, emphasizing their roles in quality assessment, performance prediction, and defect detection.

For asphalt binders, CV facilitates detailed microstructural analysis, including the evaluation of binder composition, modifier distribution, and molecular interactions. High-resolution imaging and advanced processing algorithms revealed correlations between image parameters and binder properties, providing valuable insights for material design and performance optimization [145]. CV also enhances quality control by identifying production defects, such as bubbles, cracks, and inconsistencies, ensuring formulation consistency and reliability.

In asphalt mixtures, CV examines microstructural features, such as composition distribution, aggregate shape, and binder-aggregate adhesion. These analyses inform mechanical modeling and enable the detection of defects, such as voids and irregularities, supporting both quality evaluation and design optimization [146]. Integrating image data with ML models allows for accurate prediction of mixture performance under varying environmental conditions [147]. In pavement monitoring, CV provides real-time assessment by identifying damage types, such as cracks, potholes, and surface wear, and supports quality control during construction to ensure compliance with design standards [148]. The analysis of historical image data enables the prediction of pavement deformation and degradation, improves maintenance planning, and supports pavement durability and safety.

CV integration is poised to transform asphalt research, with its full potential in asphalt omics still unfolding. Future advancements will likely emphasize real-time microstructural characterization, multiscale nondestructive detection, and automated performance monitoring, supported by advances in three-dimensional (3D) imaging, hyperspectral analysis, and robotics. Moreover, CV integration with molecular analysis techniques, such as spectroscopy and tomography, could enable precise, multiscale mapping of material composition and structure, providing deeper insights into the fundamental mechanisms governing asphalt performance.

4.4. Numerical simulation in asphalt omics

Asphalt omics relies on advanced AI for data analysis and numerical simulation tools to bridge performance prediction, virtual experimentation, and mechanistic interpretation. Among these tools, the finite element method (FEM) and discrete element method (DEM) are essential for modeling the mechanical responses, structural evolution, and environmental interactions of asphalt systems, enhancing performance prediction and supporting the optimization of omics-based design.

(1) Finite element method. The FEM discretizes continua into elements, enabling efficient solutions of partial differential equations over complex geometries. Its multiscale modeling framework effectively captures asphalt viscoelastic behavior, mixture damage, layered pavement responses, and pollutant diffusion, establishing FEM as a core numerical tool for asphalt material-structure-environment studies.

In asphalt material omics, the FEM simulates mechanical behavior by integrating rheological constitutive equations to capture responses under varying conditions, supporting structure–property analysis [149]. FEM has been applied to predict fatigue and fracture performance, enhance experimental interpretation by modeling specimen geometry and stress distribution, and inform performance-driven material design by modeling functional material distributions and stress transfer pathways [150]. However, many FEM models rely on idealized assumptions regarding homogeneity and bonding, limiting their accuracy in capturing real-world asphalt behaviors. In pavement omics, FEM simulates mixtures and layered pavement structures, analyzes the interfacial stress, particle contacts, and material interactions for design optimization. The FEM evaluates the aggregate type, gradation, and structural parameters [151], predicts stress–strain responses, fatigue cracking, rutting deformation [152], and model construction processes, such as compaction and

bonding [153-154]. In environmental omics, the FEM models multi-physical responses under temperature gradients, moisture intrusion, and solar radiation, supporting the development of sustainable pavements. Applications include analysis of flood responses, climate impacts, noise reduction, and the thermal performance of snow-melting and phase-change pavements [155], as well as modeling pollutant transport and contaminant migration in subsurface soils. Accurately capturing multiscale interactions between environmental factors and materials remains a challenge, highlighting the need for more comprehensive, data-driven FEM models.

The FEM provides a multiscale framework linking material composition, structural form, and construction behavior, facilitating the transition from empirical approaches to mechanistic understanding. Conventional analyses often assume macroscopic homogeneity, overlooking critical micro- and mesoscale effects, including crack propagation. Enhancements, such as the extended FEM incorporates discontinuous functions to more accurately simulate crack growth; the cohesive zone model defines traction-separation laws at material interfaces for improved representation; the phase-field method captures phase separation and crack growth; and the virtual crack closure technique predicts crack growth based on energy release rates, making it effective for mixed-mode fracture simulations [156].

Multiscale FEM (MsFEM) enables independent modeling across different scales, using representative volume elements to integrate microstructures with global responses [157]. MsFEM has been applied to investigate thermodynamic and cohesive properties, correlate microstructural interactions with adhesion, and capture rutting and cracking mechanisms. Furthermore, it accommodates thermal effects, such as radiative and convective heat transfer [158]. Within asphalt omics, FEM must evolve into advanced, data-driven approaches that integrate multi-physics models, microstructural descriptors, and high-throughput data to enhance parameter identification and predictive accuracy. AI-assisted FEM further enhances calibration and optimization, aligning simulations with omics principles for material design, structural evaluation, and environmental adaptation.

(2) Discrete element method. The complex, heterogeneous structure of asphalt mixtures results from the combined effects of aggregates, fillers, binders, and additives. Performance is governed by the mineral skeleton, binder rheology, and their interactions. The DEM models materials as assemblies of particles, enabling the simulation of aggregate rearrangement, binder-aggregate debonding, and gradation reconstruction. This makes DEM a powerful tool for virtual mixture design, failure mechanism analysis, and multiscale performance prediction. DEM supports asphalt mixtures design by predicting modulus across varying filler concentrations, analyzing aggregate interactions, interfacial bonding, and internal force under load. It simulates the effects of aggregate gradation, binder content, and loading speed on indirect tensile strength, closely aligning with laboratory results. Furthermore, DEM models compaction processes, indicating the impact of gradation and geometry on air voids, and predicting mechanical behavior under loads by capturing particle rearrangement, force chain formation, and modulus evolution.

Applications of DEM include simulating low-temperature behavior with viscoelastic and elastoplastic contacts, modeling surface texture evolution under repeated tire loading, and evaluating paving speed, compaction parameters, and repair strategies [159]. DEM provides insights into damage mechanisms by capturing crack initiation, propagation, and coalescence, quantifying interfacial stresses during freeze-thaw cycles, evaluating moisture damage, and modeling rate-dependent behavior [160]. Additionally, DEM simulates self-healing, micro-crack evolution, and interactions between micro- and macro-cracks under dynamic loading.

Achieving high simulation accuracy requires the reconstruction of critical material features, such as aggregate morphology and void distribution using advanced imaging techniques [161]. For example, 3D aggregate models were reconstructed using Materialize Mimics, linear contact parameters were obtained through nanoindentation, and parallel bond model parameters were determined through tensile adhesion and shear tests. Real-time calibration methods, including sensor data integration with Kalman filters, have also been explored to enhance the DEM accuracy and better represent real-world behavior. Advanced methods have been developed to further improve DEM simulations. The

discrete cohesive zone model employs a bilinear force-displacement law to capture interfacial debonding, although it primarily addresses interface behavior. The discrete damage zone model (DDZM) incorporates both interface softening and bulk stiffness degradation, providing a more comprehensive framework for modeling fiber debonding and matrix cracking [162]. Particle-based methods, such as the particle flow method, lattice Boltzmann method (LBM), and smoothed particle hydrodynamics (SPH), enable realistic simulations of particle contact, rearrangement, and fluid interactions. For example, SPH has been utilized to evaluate hydroplaning risks by modeling dynamic interactions between water films and rough textures, whereas LBM has been applied to predict permeability in asphalt mixtures by reconstructing 3D microstructures from X-ray CT scans.

The FEM, grounded in continuum mechanics, often fails to capture the multiscale and multi-phase characteristics of asphalt mixtures. It struggles to accurately represent nonlinear contact and friction, particularly at the asphalt–aggregate interface, which limits simulation accuracy. Conversely, the DEM effectively models discrete particle interactions, including contact, rolling, and sliding behaviors. However, the DEM is computationally intensive for large-scale bulk material simulation. Consequently, neither the FEM nor the DEM alone can fully characterize the complex behavior of asphalt mixtures [163]. To address these limitations, hybrid modeling approaches have been developed, integrating multiple simulation techniques to better represent complex, multiscale phenomena. Table S11 in Appendix A highlights these integrated methods, providing insights into more accurate material and structural analyses.

Hybrid modeling approaches have significantly improved simulation accuracy by capturing intricate multiscale interactions. By integrating advanced data analytics, parameter identification, data-driven calibration, and real-time prediction were further enhanced. Multi-technology frameworks integrate the macro-scale capabilities of FEM with the micro-scale precision of the DEM and other particle-based methods, whereas AI accelerates solution processes, enabling more realistic simulations. However, challenges in simulating asphalt materials and their environmental impacts persist. Incorporating MD can improve the representation of molecular-scale binder behavior, whereas coupling these models with life-cycle assessment and pollutant transport simulations can provide a more comprehensive understanding of the environmental footprint associated with asphalt production, use, and end-of-life processes.

5. Asphalt omics data platform

5.1. Data platform structure

Asphalt omics testing and analysis platforms generate extensive datasets that present significant management and analytical challenges. A robust data platform should be established to integrate diverse data sources and ensure efficient storage, processing, and analysis. Such a platform facilitates deeper insights into the relationship between asphalt microstructure and performance, driving material innovation and optimization. The database architecture is shown in Fig. S6 in Appendix A.

(1) **Data acquisition layer.** This foundational layer utilizes advanced instrumentation to capture raw data on chemical composition, physical properties, and performance metrics. Standardizing data collection across instruments and data types ensures compatibility and accuracy, minimizes discrepancies, and enables seamless integration into subsequent processes.

(2) **Data storage layer.** Leveraging efficient database management systems—including relational databases (e.g., MySQL (Oracle Corporation, USA), PostgreSQL (PostgreSQL Global Development Group, USA)) and NoSQL databases (e.g., MongoDB (MongoDB Inc., USA))—this layer stores large datasets in standardized formats to ensure consistency and facilitate cross-disciplinary collaboration. Real-time interaction capabilities and caching technologies provide high availability and low latency.

(3) **Data processing layer.** This layer preprocesses raw data, including data cleaning, missing-value imputation,

and outlier detection to enhance data quality. It also standardizes processed data to satisfy the requirements of various analytical methods. A flexible processing pipeline supports the adaptation of workflows to accommodate the diverse analytical requirements of omics technologies.

(4) Data analysis layer. This layer leverages statistical analysis, chemometrics, and AI to perform comprehensive analyses and builds predictive models to uncover patterns and relationships, aiding in optimizing material performance and developing novel materials. Key requirements include the capacity to process extensive datasets and provide flexibility and scalability, enabling researchers to adapt analyses as research progresses.

(5) Data visualization layer. This layer presents the analytical results visually using tools, such as Tableau (Tableau Software LLC, USA), Power BI (Microsoft Corporation, USA), and Grafana (Grafana Labs, USA), highlighting trends and predictive insights in asphalt materials. An intuitive user interface enables customized report generation, enabling the automatic creation of tailored analytical reports to enhance research efficiency and usability.

To achieve standardized construction and sharing of an asphalt omics database, a multi-level data standard system should be established, encompassing terminology, metadata, structural specifications, and interface protocols. NLP can automate the extraction of key terms and relationships from literature and reports, supporting dedicated ontologies and metadata models to resolve semantic inconsistencies. MAS coordinates collaboration among laboratories and edge devices, ensuring standardized data acquisition and formatting consistency [164]. KGs transform multi-source data into structured representations, linking composition, performance, and environmental effects, to enable semantic search and intelligent recommendations. Federated learning supports joint model training while preserving data privacy, promoting secure and scalable data sharing across platforms [165]. Robust quality control, including rule engines and automated annotations, ensures data reliability by detecting and correcting missing or inconsistent information. These technologies enable effective data management and foster interdisciplinary collaboration in asphalt research.

Developing asphalt omics databases must address ethical and legal challenges associated with data sharing [166]. As these databases expand to incorporate diverse data from institutes, industries, and field projects, establishing a robust governance framework is essential. Key elements include clearly defined ownership and usage rights through standardized licensing, implementation of anonymization and privacy-preserving measures, tiered access controls, and enforcement of legally binding data usage protocols. Policy-level initiatives, such as international data-sharing agreements, open-access funding, and enhanced public infrastructure, are also vital for fostering a sustainable and trustworthy data ecosystem [167]. Ultimately, the objective is to create a mutually beneficial framework that advances innovation in asphalt materials science and intelligent pavement engineering.

5.2 Asphalt-related databases

Asphalt material databases aggregate critical data on rheological and mechanical performance across various types, grades, and regions. They also capture mixture performance metrics, including volumetric indicators, gradations, and material classifications. Pavement databases document the usage and performance of pavements, including distress modes, such as rutting, cracking, and delamination, to inform maintenance strategies. Data on modified, recycled, and environmentally friendly asphalt materials are frequently included.

In the United States, the Strategic Highway Research Program established key databases, such as Witczak and Long-Term Pavement Performance databases, which have been instrumental in developing predictive models, such as the dynamic modulus (E^*) [168]. The Witczak database initially comprised 41 mixtures characterized by parameters, such as viscosity and effective asphalt volume (V_{beff}), and has since expanded over time to enhance accuracy under extreme conditions and aging. In the 1990s, a nonlinear S-shaped function was introduced to more accurately characterize aged asphalt, highlighting air voids, shear modulus, viscosity, and phase angle as sensitive indicators. More

Advancements in data analysis has expanded historical databases, such as the “Master North Carolina State University (NCSU, USA)” database, which integrates data from multiple sources, such as the NCSU, Witczak database (University of Maryland, USA), Federal Highway Administration (FHWA, USA), Western Research Institute (USA), and Citgo databases (CITGO Petroleum Corporation, USA). These databases encompass a wide range of binders and aging conditions under standardized test protocols. The key asphalt material databases used worldwide are listed in Table S12 in Appendix A. However, many countries still lack dedicated databases, relying primarily on project records and reports.

Furthermore, specialized asphalt databases have been developed. For example, Yu et al. [170] developed a long-term performance database for semi-rigid asphalt pavements, whereas Chang et al. [171] established a VOC fingerprint database for asphalt materials. The details of these and other key databases are listed in Table S13 in Appendix A.

Despite these advancements, asphalt databases face persistent challenges, including limited data volume, infrequent updates, restricted access, and user-unfriendly interfaces, which impede effective data utilization and mining. The absence of standardized formats and testing methods complicates data sharing and comparison, with inconsistencies in time definitions, input parameters, and conventions. For example, the Witczak model for predicting dynamic modulus $|E^*|$ requires specific binder inputs at defined temperatures and frequencies. Most databases lack detailed information on SARA components and microchemical compositions, as asphalt origin or grade alone is insufficient for reliable identification. Although current databases focus on material properties and performance, future systems should integrate microscopic compositional and structural data from chemical analyses and imaging. Incorporating AI-driven analysis of spectra and images can provide deeper insights into the molecular characteristics of asphalt and enhance material behavior predictions.

Beyond technology, the asphalt omics database offers a substantial economic advantages [172]. Integrating high-throughput data enables more accurate material design and performance prediction. For asphalt materials, data-driven approaches minimize repetitive testing and reduce development costs. In pavement applications, asphalt omics can eliminate trial and error in empirical design, support cost-effective maintenance through long-term performance tracking, and extend service life. For pavement environments, the database quantifies the environmental impacts and informs the optimization of green materials and sustainable construction. In summary, an asphalt omics database not only advances material design and pavement management but also provides critical data to support government policy, industrial investment, and sustainability initiatives, thereby improving the economic efficiency of road engineering [173].

The ultimate objective of developing an asphalt omics database is to facilitate the intelligent and automated transformations in the asphalt industry. By providing multiscale, data-driven insights, it enables informed decision-making across the entire chain—from material design and production to construction and maintenance—enabling the transition to Road Industry 4.0. Manufacturers and contractors are adopting intelligent solutions. For example, smart asphalt mixture production systems integrate temperature monitoring, feeder control, and real-time feedback to optimize mixing, thereby improving quality and efficiency. Intelligent pavement and compaction technologies employ real-time feedback from temperature, thickness, vibration, and positioning to control layer thickness, surface smoothness, and compaction. Intelligent pavement management systems utilize monitoring data to evaluate pavement conditions and inform maintenance strategies through performance-based modeling. However, current systems still depend on sensor feedback and manual adjustments, involving experiential dependence and delayed responses. Enhanced integration of analytical platforms and robust databases is expected to enable future systems to achieve real-time data fusion, autonomous decision-making, and dynamic control through predictive models, creating automated closed-loop systems that reduce human intervention and improve consistency and efficiency.

Asphalt omics is not simply a borrowed terminology from life sciences; it represents a systematic, data-driven methodology tailored to the complexities of asphalt materials. Rather than directly transferring concepts, this approach integrates high-throughput testing, advanced computational techniques, and multiscale modeling to elucidate composition–structure–performance relationships specific to asphalt. This framework aims to move beyond descriptive analyses toward predictive, mechanistic understanding and optimized material design, thereby establishing an independent knowledge framework that satisfies the evolving demands of road engineering.

(1) Asphalt omics has been the foundation for asphalt research, encompassing fingerprinting, fractionation, and mixture design programming. These methods reflect core omics principles by developing fingerprint databases, correlating material components with performance, and enabling material design through parameter optimization. However, current approaches remain fragmented, with limited cross-scale integration. Systematically analyzing the relationships among the functional units, microstructure, and performance—leveraging precise characterization and big data—offers significant potential for advancing asphalt science.

(2) Asphalt omics conceptualizes microscopic components as fundamental functional units, utilizing high-throughput testing and intelligent data processing to elucidate the influence of these units on performance and interaction with the composition, microstructure, performance, and environmental factors. This framework enables optimized material design, drives functional material innovation, and accelerates advancements in road science.

(3) Asphalt omics operates across three interconnected levels. Material omics investigates functional units and material performance to support material development and optimization. Pavement omics examines the design parameters, construction methods, and long-term performance to enhance road design and maintenance efficiency. Environmental omics addresses road-related pollutants and fosters low-carbon, economically friendly transportation. Fully leveraging these levels requires integrating data across spatial scales (nano to macro) and temporal scales (instantaneous to long-term), and developing unified characterization models to capture multi-level interactions.

(4) Asphalt omics relies on three core platforms. The testing platform captures high-throughput data, necessitating standardized data formats for compatibility. The analysis platform leverages AI and simulation but requires improved algorithm adaptability and interpretability. The data platform consolidates results, yet faces challenges, such as limited data volume, infrequent updates, and incomplete information. Fully realizing the potential of these platforms requires long-term monitoring, enhanced analysis of complex compositions, and efficient data integration to address data scarcity, information gaps, and multi-source data fusion.

7. Outlook

Asphalt omics provides an innovative framework for advancing asphalt material development and application, yet several challenges persist. The highly heterogeneous, nonlinear, and non-biological nature of asphalt complicates accurate characterization, testing, and modeling. Testing platforms lack standardized protocols and high-throughput capabilities, resulting in inconsistent and non-comparable data. Analysis platforms require intelligent algorithms tailored to the multiscale complexity of asphalt with enhanced adaptability and interpretability. Data platforms are hindered by limited data volumes, fragmented information, and infrequent updates, impeding comprehensive data integration.

Addressing these challenges requires coordinated top-level design and bottom-level implementation. Testing platforms should adopt standardized, high-throughput procedures for consistent data collection. Analytical platforms must develop cross-domain, interpretable models to capture multiscale interactions. Data platforms must integrate diverse, heterogeneous data sources to minimize fragmentation. In practice, asphalt omics should incorporate

environmental adaptability and sustainability metrics into material design, structural optimization, and life cycle management, establishing a material-structure-environment design framework. This approach should be supported by intelligent sensing, automated construction, and carbon accounting technologies. Finally, supportive regulations and policies are essential for promoting asphalt omics and accelerating the standardized application of technological outcomes.

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Declaration of Interest Statement

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.