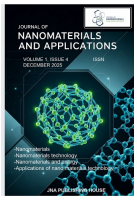
JOURNAL OF NANOMATERIALS AND APPLICATIONS

Journal of Nanomaterials and Applications

Journal homepage: https://jna.com.vn



The power of simulation: Exploring binary alloys for next-generation applications

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Review info

Type of paper:
Review article

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Received: 27 September 2025
Revised: 23 October 2025
Accepted: 24 October 2025
Published: 30 October 2025

Abstract: This review provides an updated perspective on the transformative role of computational simulation in the design and discovery of binary alloys for advanced technologies. Unlike traditional trial and error methods, molecular dynamics (MD) and density functional theory (DFT) simulations now deliver atomistic insights into structure property relationships, enabling more predictive materials design. Recent developments demonstrate that hybrid strategies integrating DFT, MD, machine learning (ML), and multiscale modeling are accelerating the discovery of high performance alloys. The article emphasizes the novelty of simulation-driven design frameworks while identifying critical research challenges, including scalability, force-field accuracy, and the integration of simulation with digital twin concepts. Through selected case studies ranging from semiconductors and biocompatible biomedical alloys to energy materials and emerging 2D binary systems this review argues that computational simulation is shifting from a supplementary role to a central driver of innovation in modern materials science.

Keywords: Binary Alloys; Computational Simulation; Molecular Dynamics; Density Functional Theory; Machine Learning.

1. Introduction

The discovery and rational design of advanced functional materials constitute a cornerstone of technological innovation in the twenty first century. Among these, binary alloys comprising two constituent elements represent one of the most fundamental yet versatile material classes, owing to their tunable structural, electronic, and thermal properties. Their technological significance spans a broad range of applications, including aerospace engineering, semiconductor devices, energy storage,

heterogeneous catalysis, and biomedical systems [1]. Historically, alloy development has been dominated by labor-intensive experimental methodologies based on iterative synthesis and characterization. While effective, such trial and error approaches demand extensive time and resources and are increasingly misaligned with the accelerating demand for materials tailored to next-generation technologies such as renewable energy platforms, quantum devices, and precision medicine [2]. In response, computational simulation has emerged as a paradigm-shifting framework for materials discovery. Enabled by advances in high performance computing (HPC), graphics processing unit (GPU) acceleration, and artificial intelligence (AI), simulations are now capable of probing atomistic interactions and predicting emergent macroscopic behaviors prior to experimental realization [3]. Central to these developments are quantum-mechanical methods such as density functional theory (DFT), which achieve an effective balance between predictive accuracy and computational tractability [4]. Complementarily, molecular dynamics (MD) simulations provide a dynamic perspective, enabling the exploration of temperature-dependent and time evolving phenomena in complex alloy systems [5]. Recent simulation-based studies have further substantiated these advantages, demonstrating how molecular dynamics and first-principles approaches can elucidate crystallization mechanisms, phase transitions, and electronic properties in representative binary systems such as Au–Cu, Ag–Au, Ni–Au, and W–Si alloys [6–11]. These investigations confirm the predictive capability of atomistic simulations in capturing microstructural evolution and thermodynamic behavior, thereby bridging the gap between theoretical modeling and experimental observation. The integration of data-driven methodologies has further amplified these capabilities. Machine learning (ML) and deep learning (DL) algorithms, when coupled with high-dimensional materials descriptors and advanced feature-selection techniques, have demonstrated the capacity to uncover latent structure property relationships beyond the reach of conventional analysis. Notably, supervised learning models such as random forests, support vector machines, and neural networks have been successfully applied to predict phase stability, mechanical resilience, and thermal transport properties in binary and multicomponent alloy systems [12–14]. Large-scale initiatives in materials informatics have provided the essential data infrastructure for these advances. Resources such as the Materials Genome Initiative (MGI), the Novel Materials Discovery (NOMAD) repository, the Open Knowledgebase of Interatomic Models (OpenKIM), and Automatic Flow for Materials Discovery Library (AFLOWLIB) offer extensive datasets encompassing DFT-calculated properties, crystallographic structures, elastic constants, and more [15–18]. These repositories, coupled with high-throughput computational frameworks such as AFLOW and the Materials Project, have dramatically expanded the accessible design space for binary alloys, facilitating inverse design strategies and rapid screening of candidate materials [16, 17]. Nevertheless, significant challenges persist. Real-world binary alloys exhibit complexities compositional disorder, interfacial phenomena, kinetic constraints that are not fully captured by idealized computational models. Furthermore, ensuring the transferability of ML models trained on curated datasets to realistic processing environments remains an open problem [19]. To address these limitations, the integration of first-principles modeling with machine learning, multiscale simulation, and uncertainty quantification is increasingly recognized as essential for achieving robust and generalizable predictions [20]. Taken together, the accelerated discovery of binary alloys through the synergy of computational simulation, AI, and informatics heralds a transformative shift in materials science. By compressing design cycles from decades to mere months or even weeks this paradigm offers unprecedented opportunities for meeting urgent global challenges, including energy sustainability,

decarbonization, and the development of next-generation electronic and biomedical technologies [21]. The following sections examine the computational methodologies, data infrastructures, machine learning frameworks, and application domains that underpin this emerging approach to alloy discovery. The content of this article focuses on focus on research and point out the role of simulation in the research process, synthesizing binary alloys to show that in addition to experimental methods, theoretical methods, simulation methods play a very important role in the research process. With outstanding advantages such as quick survey, giving quite accurate results, creating a solid foundation for future experimental processes. With the MD method used when researching the structure, phase transition process of materials with large atomic numbers in the temperature region greater than room temperature (a harsh region that experiments cannot reach), fast research while the DFT method researches with materials with quantum structures of only a few dozen atoms, 0K temperature region, slow research requires a server with a quantum computer configuration.

2. Fundamentals of computational simulation methods

Computational methodologies have become integral to contemporary materials science, playing a pivotal role in the accelerated discovery and design of binary alloys. These approaches provide unparalleled insights into atomic-scale interactions, phase evolution, and electronic structure, offering predictive capabilities that complement and often surpass traditional experimental techniques. Central to this computational toolkit are MD, DFT, and hybrid strategies that integrate multiscale modeling with machine learning. This section presents an overview of their theoretical foundations, current methodological advances, and key applications in the study and engineering of binary alloy systems.

2.1. Molecular dynamics.

Molecular dynamics (MD) provides a computational framework for simulating the temporal evolution of atomic systems through numerical integration of Newton's equations of motion, offering detailed insights into material behavior over nanosecond to microsecond timescales [22]. This methodology relies on predefined interatomic potentials, such as Embedded Atom Method (EAM), Modified Embedded Atom Method (MEAM), and Tersoff potentials, and is particularly effective for capturing thermally activated phenomena, including diffusion, grain boundary migration, dislocation dynamics, phase transformations, and mechanical deformation in binary alloys [23]. Recent advances in GPU-accelerated MD packages, including Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), GROningen MAchine for Chemical Simulations (GROMACS), and Open Molecular Mechanics (OpenMM), have dramatically expanded the accessible simulation scale, enabling the study of systems containing millions of atoms within computationally feasible times [24]. These developments have facilitated large-scale investigations of polycrystalline binary alloys, allowing accurate predictions of melting behavior, grain boundary sliding, and crack propagation under applied mechanical loads [25]. Between 2022 and 2024, multiple studies highlighted the capability of MD to model alloy responses under extreme conditions. Shock compression simulations of Ni–Al and Cu–Zr alloys successfully reproduced experimentally observed Hugoniot curves, while ultrafast laser heating studies elucidated nanoscale thermal transport mechanisms relevant to additive manufacturing [26, 27]. Furthermore, the emergence of machine-learned force fields, including Moment Tensor Potentials (MTP) and Neural Network Potentials, has significantly enhanced the predictive accuracy of MD simulations, approaching the fidelity of first principles calculations [25].

2.2. Density functional theory

Density Functional Theory (DFT) is a quantum-mechanical framework that treats the electron density as the central variable, providing an approximate solution to the many-body Schrödinger equation via the Kohn–Sham formalism [28]. DFT is highly effective in predicting ground-state properties of crystalline systems, including lattice parameters, cohesive energies, bulk moduli, electronic band structures, magnetic ordering, and vibrational spectra [29]. In the study of binary alloys, DFT has become indispensable for calculating formation enthalpies, electronic density of states (DOS), phase diagrams, and elastic constants, offering critical insights into phase stability, solute interactions, and miscibility gaps parameters essential for rational alloy design [23]. Beyond equilibrium structures, DFT enables the exploration of metastable or high-pressure phases that are often inaccessible to experimental characterization [22]. Recent methodological advancements, including hybrid functionals (e.g., Heyd–Scuseria–Ernzerhof 2006 (HSE06)), Green's function and screened Coulomb interaction (GW) corrections, and Time-Dependent Density Functional Theory (TD-DFT), have expanded the predictive scope to electronic band gaps and optical properties, facilitating the study of semiconductor and optoelectronic alloys such as Si–Ge, In–Ga, and Sn–Se systems [24, 27]. Spin-polarized DFT calculations have further enabled the investigation of magnetic binary alloys (e.g., Fe–Pt, Co–Ni), supporting the design of materials for data storage and spintronic applications [29].

2.3. Hybrid approaches

Despite the considerable capabilities of individual computational approaches, each method exhibits intrinsic limitations: MD lacks quantum-level accuracy, whereas DFT becomes computationally prohibitive for large or complex systems. To overcome these constraints, hybrid strategies that synergistically integrate complementary methodologies have gained prominence in alloy modeling. A widely employed approach is DFT-informed MD, wherein interatomic potentials for MD simulations are parameterized using DFT-derived data, thereby ensuring fidelity in bonding behavior, defect energetics, and thermodynamic predictions [25]. Machine learning (ML) potentials trained on high-fidelity DFT or MD datasets such as MTP and Gaussian Approximation Potentials (GAP) offer a compelling compromise between predictive accuracy and computational efficiency [25, 26]. Multiscale modeling frameworks further extend this integration by coupling atomistic simulations with continuum level methods, including phase-field modeling and finite element analysis, enabling the bridging of temporal and spatial scales essential for simulating alloy solidification, coarsening, and microstructural deformation [1]. Recent AI-enhanced strategies leverage high-throughput DFT or MD data within ML pipelines to rapidly explore extensive compositional spaces. Convolutional neural networks (CNNs) and graph based architectures, such as Crystal Graph Convolutional Networks (CGCNN), have been successfully applied to predict formation energies, mechanical hardness, and corrosion resistance across vast binary alloy systems [23]. As materials science increasingly embraces inverse design and autonomous discovery paradigms, these hybrid methodologies are poised to drive next generation alloy development. By combining the quantitative rigor of quantum mechanics, the scalability of classical simulations, and the pattern recognition power of AI, they enable accurate, efficient, and previously unattainable exploration of complex alloy design spaces [27]. However, each method presents its own challenges. With the experimental method, the biggest challenge is that the material size must be larger than 2nm or the research temperature must be below 4000 K because the measuring equipment used for research cannot access it. With the simulation method, it is impossible to access too large a number of atoms. Too large a

number of atoms will greatly affect the processing speed of the server. This is the biggest limitation of the simulation method, increasing the calculation time. To solve these problems, each method will choose the conditions to optimize the research process. The results are determined by approximate methods to determine the results to ensure that the results are close to the experiment.

3. Simulation driven discovery and optimization of binary alloys

Computational simulation has fundamentally reshaped the discovery, characterization, and optimization of binary alloys, establishing itself as a cornerstone of modern materials science. By providing a virtual laboratory, atomistic and quantum-level modeling techniques allow unprecedented access to the intricate structure property relationships that govern material behavior across compositional, phase, and microstructural dimensions. These methodologies enable researchers to probe phenomena that are often inaccessible or challenging to measure experimentally, including defect energetics, atomic diffusion pathways, phase stability under extreme conditions, and nanoscale mechanical responses. Beyond offering predictive insights, simulation significantly reduces the dependence on labor-intensive trial and error experimental workflows, thereby compressing the traditional materials design cycle from years or decades to mere months. This acceleration is particularly valuable for the development of application-specific alloys, where targeted optimization of electronic, thermal, mechanical, or magnetic properties is critical. For instance, simulations can guide the selection of alloying elements to enhance corrosion resistance in biomedical implants, improve high-temperature stability in aerospace components, or tailor band structures in semiconductor alloys [30]. Moreover, the integration of simulation with high throughput computational screening, machine learning, and multiscale modeling has expanded the accessible design space for binary alloys, enabling systematic exploration of previously intractable compositional and structural combinations. As a result, simulation-driven alloy discovery is transitioning from a supplementary tool to a directive framework, providing not only mechanistic understanding but also actionable guidance for rational materials engineering and next generation technology development.

To ensure reliability, the process of alloy discovery by simulation always requires cross-validation with experimental data. Studies have demonstrated that predictions from atomistic simulations can successfully reproduce observed macroscopic quantities: Mechanical predictions: MD simulations of shock compression of Ni–Al and Cu–Zr alloys successfully reproduced the experimentally observed Hugoniot curve. Electronic structure predictions: DFT and GW calculations of Si–Ge alloys predicted reduced band gap and carrier mobility, which were confirmed in epitaxial thin films.

3.1. Mechanical properties.

MD simulations have provided profound insights into the atomic-scale mechanisms governing plastic deformation, dislocation nucleation and motion, twinning, and grain boundary evolution in binary alloys [31]. By resolving the temporal and spatial evolution of atoms under applied stress or thermal fluctuations, MD enables the direct observation of phenomena that are challenging to capture experimentally, offering mechanistic understanding essential for materials design. For instance, in Ti–Nb and Cu–Zn alloy systems, solute atoms have been shown to significantly influence stacking fault energies and slip behavior, thereby modulating ductility, deformation modes, and work-hardening characteristics [32, 33]. Specifically, in Ti–Nb alloys widely utilized in orthopedic implants combined MD and DFT studies demonstrate that Nb additions suppress α’ -martensitic transformations while stabilizing the β-phase, allowing precise tuning of the elastic modulus and facilitating transformation-induced plasticity (TRIP) effects that enhance mechanical performance under physiological loading [34]. Recent advances

integrating machine learning with MD simulations have further expanded the scope of alloy design. ML augmented MD frameworks enable high-throughput compositional screening, identifying binary alloys with optimized mechanical properties. Notably, studies on Al–Mg and Fe–Ni systems have revealed compositions exhibiting enhanced toughness, grain-boundary strengthening, and high-strength characteristics, features particularly relevant for demanding aerospace and structural applications [35, 36]. These developments underscore the growing role of MD, not only as a tool for mechanistic exploration but also as a predictive platform for rational alloy engineering.

3.2. Thermal properties

Thermal transport in binary alloys is largely governed by phonon scattering arising from mass disorder, bond inhomogeneity, and lattice imperfections. First-principles approaches, particularly DFT combined with phonon dispersion calculations and Boltzmann Transport Equation (BTE) solvers, have been successfully applied to systems such as Si–Ge and Al–Mg alloys, providing quantitative predictions of reduced phonon mean free paths and suppressed lattice thermal conductivity [37, 38]. These calculations elucidate the fundamental mechanisms by which compositional complexity and interatomic bonding variations impede heat flow, enabling the rational design of alloys for thermoelectric or heat-management applications. MD simulations offer a complementary perspective by inherently capturing anharmonic effects, temperature-dependent scattering processes, and interfacial thermal resistance. Recent MD studies on Fe–Ni alloys have demonstrated that short-range order (SRO) and local atomic arrangements can substantially modify phonon lifetimes, enhancing thermal stability and mechanical resilience at elevated temperatures [39]. By combining DFT–BTE predictions with atomistic MD insights, researchers can achieve a multiscale understanding of thermal transport, bridging the gap between fundamental lattice dynamics and macroscopic thermal behavior. Such integrative modeling frameworks are increasingly critical for designing binary alloys in high temperature, energy, and electronic applications, where precise control over heat conduction is essential for performance and reliability.

3.3. Electronic properties

DFT has become a cornerstone in the investigation of electronic band structures in semiconducting binary alloys. In systems such as Si–Ge and Bi–Sb, first-principles simulations have demonstrated that both band gap energies and carrier mobilities can be systematically tuned through compositional variation, atomic ordering, and applied strain, providing critical guidance for the design of high-performance electronic devices [40, 41]. Layered transition metal dichalcogenide alloys, such as MoS_2-WS_2, further illustrate the sensitivity of electronic properties to structural configuration. In these materials, the stacking sequence and alloy composition dictate the band gap, which spans a range from approximately 1.2 to 1.9 eV, directly influencing their suitability for optoelectronic, photonic, and valleytronic applications [42]. Beyond conventional DFT, advanced techniques such as the GW approximation and time dependent DFT (TD-DFT) have been employed to capture excitonic effects and interband transitions, enabling more accurate predictions of light absorption, photoluminescence, and optical response spectra [43]. Complementing these quantum mechanical approaches, machine learning (ML) models trained on extensive DFT datasets have facilitated high throughput screening and accelerated exploration of previously uncharted compositional spaces, thereby identifying promising candidate semiconductors with targeted electronic properties [44].

3.4. Energy-related applications

Binary alloys have emerged as highly promising candidates for energy storage and conversion

applications, owing to their tunable composition dependent properties and structural versatility. First principles studies indicate that Al–Mg alloys possess favorable hydride formation enthalpies, making them attractive as lightweight hydrogen storage media with high gravimetric and volumetric capacities [45]. In Fe–Ni systems, computational investigations have demonstrated that optimizing the nickel content can enhance corrosion resistance, catalytic performance, and structural stability, rendering these alloys particularly suitable for solid oxide fuel cell (SOFC) components [46]. In the context of lithium-ion batteries, Si–Sn and Sn–Sb alloys have been extensively studied using combined Molecular Dynamics (MD) and DFT approaches. These simulations reveal that alloy composition critically influences lithium-ion diffusion pathways, volumetric expansion during lithiation, and overall cycling stability, providing mechanistic insights that inform the design of next-generation anode materials [47]. Moreover, the integration of artificial intelligence (AI) with high-throughput DFT screening has facilitated the discovery of novel binary alloy catalysts for electrochemical CO_2 reduction and ammonia synthesis. By rapidly evaluating vast compositional spaces and predicting key catalytic descriptors, these AI-assisted strategies exemplify the synergistic potential of combining atomistic modeling and machine learning to accelerate the development of sustainable energy materials [48]. Collectively, these studies underscore the central role of computationally guided alloy design in addressing critical challenges in energy storage, conversion, and sustainable technology development.

4. Case studies simulation in action

Computational simulation exemplifies the translational potential of modern materials modeling, bridging the gap between theoretical predictions and experimental realization, as well as facilitating subsequent industrial integration. Representative studies across diverse alloy systems demonstrate how atomistic and quantum-level simulations can directly inform materials design: guiding the development of semiconducting alloys with tailored electronic properties, optimizing biomedical alloys for mechanical performance and biocompatibility, engineering structural alloys with enhanced strength and ductility, and enabling nanoscale design in advanced electronic and optoelectronic devices. These examples collectively underscore the capacity of computational approaches to accelerate the discovery to application pipeline, transforming abstract modeling insights into tangible technological advancements.

4.1. High-performance semiconductor materials (Si–Ge)

The Si–Ge binary alloy system serves as a canonical example of how computational simulations can directly influence the development and optimization of semiconductor technologies. SiGe alloys play a pivotal role in complementary metal oxide semiconductor (CMOS) transistors, infrared detectors, and thermoelectric devices, owing to their tunable band gaps and enhanced carrier mobility relative to pure silicon [40]. First principles DFT calculations, complemented by GW corrections, have systematically mapped the correlation between germanium concentration and electronic band structure, revealing a band gap reduction from 1.12 eV in pure Si to approximately 0.66 eV in pure Ge [49]. Strain-engineering simulations have further elucidated the modulation of band curvature and mobility anisotropy, predictions that have been experimentally validated in epitaxial thin films [50]. MD studies provide atomistic insights into defect formation, interdiffusion, and thermal transport in SiGe heterostructures, informing strategies for precise control of epitaxial growth. Coupled DFT–MD investigations have guided the design of SiGe nanowires and superlattices, enabling the realization of experimental thermoelectric figure-of-merit (ZT) values exceeding 1.5 [51]. Collectively, these computational advances have facilitated the direct translation of theoretical insights into industrial practice, exemplified by the

integration of strain-engineered Silicon Germanium (SiGe) channels in advanced Fin Field Effect Transistor (FinFET) nodes deployed by leading semiconductor manufacturers such as Intel [52]. This case underscores the capacity of simulation driven design to accelerate both fundamental understanding and technological deployment in high-performance electronic materials.

4.2. Biocompatible biomedical materials (Ti–Nb)

The Ti–Nb binary alloy system has emerged as a leading candidate for orthopedic implant applications due to its exceptional biocompatibility, corrosion resistance, and highly tunable elastic modulus. DFT investigations have demonstrated that Nb additions effectively stabilize the β-phase of titanium, reducing the elastic modulus from approximately 110 GPa in pure Ti to 40–60 GPa, closely matching the mechanical properties of cortical bone and minimizing stress shielding effects [32]. MD simulations provide mechanistic insight into the role of Nb in governing dislocation motion, twin boundary formation, and defect mediated plasticity, elucidating the origins of enhanced fatigue resistance under cyclic loading conditions [53]. Surface level ab initio molecular dynamics (AIMD) calculations further reveal favorable adsorption energetics for hydroxyapatite, supporting osteointegration and highlighting the potential for improved bone implant interface performance [54]. Recent advances in multiscale modeling have integrated atomistic simulations with additive manufacturing (AM) process parameters, predicting how powder bed fusion (PBF) conditions influence porosity, microstructural evolution, and martensitic transformation in Ti–Nb alloys. These simulations enable the rational optimization of AM processing routes to produce implants with tailored mechanical properties and reliable in vivo performance [55]. Collectively, these computational studies illustrate how integrated simulation frameworks can accelerate the design, fabrication, and clinical translation of next generation biomedical alloys.

4.3. Lightweight structural alloys (Al–Mg)

Al–Mg binary alloys occupy a central role in lightweight structural engineering due to their high specific strength, corrosion resistance, and formability. DFT studies of Al–Mg phase diagrams have elucidated the stability ranges of solid solutions and intermetallic compounds, such as β-Al_3Mg_2, providing essential guidance for alloy design aimed at mitigating embrittlement and enhancing mechanical reliability [56]. MD simulations have offered atomistic insights into the influence of magnesium on dislocation density, grain boundary cohesion, and impact resistance, revealing mechanisms of mechanical strengthening and energy absorption at the nanoscale [57]. Coupled with simulation-informed precipitation studies, these approaches have enabled the optimization of heat treatment schedules, which have been experimentally validated in Al–Mg–Si alloy systems to achieve controlled microstructures and enhanced mechanical performance [38]. At larger scales, finite element models parameterized using MD-derived constitutive data allow accurate prediction of crash and impact behavior in Al–Mg sheet components, substantially reducing reliance on costly experimental testing [58]. Recent developments integrating machine learning (ML) with DFT datasets have further accelerated high-throughput screening of Al–Mg compositions, enabling the identification of alloys with superior resistance to corrosion and hydrogen embrittlement, a key consideration for lightweight and safe electric vehicle housings [59]. Collectively, these computational strategies demonstrate the multiscale potential of simulation-driven alloy design, bridging atomic insights to structural performance and industrial implementation.

4.4. 2D binary alloys for nanoelectronics (MoS_2–WS_2, graphene–hBN)

Two-dimensional (2D) binary alloys represent a frontier in computational materials design, with

significant implications for nanoelectronics, optoelectronics, and flexible device technologies. DFT calculations indicate that MoS_2–WS_2 alloys maintain direct band gaps tunable between 1.5 and 1.9 eV, rendering them highly suitable for applications in optoelectronic devices, photodetectors, and valleytronic architectures [42]. Monte Carlo simulations combined with cluster expansion techniques have revealed the thermodynamic stability of short-range ordering and domain size distributions, which are critical parameters for controlling growth quality during chemical vapor deposition (CVD) synthesis [60]. Similarly, graphene–hBN hybrid alloys (CBN materials) exhibit compositionally tunable electronic band gaps spanning 0–5.5 eV, as predicted by hybrid DFT studies, providing design flexibility for semiconducting and insulating components in nanoscale electronics [61]. MD simulations complement these insights by evaluating thermal transport, mechanical response, and structural stability under applied strain, essential for the reliable integration of these 2D alloys into flexible and stretchable electronic devices [62]. Recent advances in predictive modeling of nucleation energetics and interlayer interactions have further guided the experimental realization of van der Waals heterostructures, demonstrating how computational design can bridge fundamental theory with practical fabrication and device implementation [63]. Collectively, these studies underscore the transformative role of simulation in advancing 2D binary alloys from theoretical prediction to technological deployment.

5. Challenges and future prospects

Despite significant progress in simulation-driven alloy discovery, several critical challenges remain that limit the full scale deployment and integration of computational predictions into experimental and industrial workflows. These challenges stem from both methodological limitations and gaps in computational and experimental infrastructure, necessitating coordinated efforts across the materials modeling, data science, and experimental communities. The challenging problem of simulation method not only exists in the potential force field but also exists in the implementation method, model size and many other limitations that have not been thoroughly resolved.

5.1. Persistent challenges

(i) Force field accuracy in MD: The predictive reliability of MD simulations critically depends on the accuracy of the underlying interatomic potentials. Classical empirical force fields, such as Embedded Atom Method (EAM) or Modified Embedded Atom Method (MEAM), offer computational efficiency but often fail to capture complex bonding environments accurately, particularly in alloys exhibiting charge transfer, magnetic interactions, or pronounced anharmonic effects. Consequently, predictions of defect energetics, surface diffusion, or phase transformations in systems with mixed bonding character such as Al–Mg and Fe–Ni alloys remain limited when relying solely on classical potentials [64, 65]. Recent developments in machine-learned potentials, including Moment Tensor Potentials (MTP) and Neural Network Potentials (NNP), show promise in bridging this gap, but widespread adoption and validation across diverse binary alloys remain ongoing challenges.

(ii) Computational scaling of DFT: While DFT provides high fidelity predictions of electronic structure, energetics, and thermodynamic properties, its computational cost scales steeply with system size and electron count, typically as $\sim O(N^3)$. This restricts practical DFT applications to relatively small unit cells and low defect concentrations. Although linear-scaling methods, GPU acceleration, and high throughput frameworks have extended the feasible problem size, large scale simulations involving long-timescale dynamics, high temperature phase evolution, or multicomponent systems remain computationally prohibitive for many binary alloys [17, 66].

(iii) Limited integration between simulations and experiments: Despite the sophistication of computational methods, their full potential is often unrealized due to insufficient integration with experimental workflows. Disparities in data formats, lack of standardized metadata, and the absence of real-time feedback loops impede validation, iterative refinement, and the translation of predictions into practical alloy design. Furthermore, simulations frequently assume idealized conditions perfect crystals at 0 K whereas real world materials contain grain boundaries, impurities, and coupled multi physics interactions. Closing this gap is essential for enabling predictive, experiment informed simulation pipelines capable of guiding the design, fabrication, and deployment of advanced binary alloys [15, 67]. The biggest challenge for ML is the quality, variety, and coverage of the dataset. Most large data repositories such as the Materials Project or NOMAD are based primarily on ground-state (0 K) DFT calculations, which creates a large data gap for properties at nonequilibrium, high temperatures, or realistic processing conditions (e.g., cooling rates, thermal gradients). This makes the transferability of ML models to real-world processing environments difficult.

5.2. Emerging solutions and opportunities

5.2.1. Machine learning-driven force fields

Machine learning interatomic potentials (MLIPs), including the Gaussian Approximation Potential (GAP), Spectral Neighbor Analysis Potential (SNAP), and Moment Tensor Potential (MTP), constitute a transformative advance in MD simulations. By training on extensive DFT datasets, these potentials achieve near quantum mechanical accuracy while maintaining the computational efficiency of classical MD. MLIPs have been successfully employed to model complex phenomena such as dislocation nucleation and motion, crack initiation and propagation, and phase transitions in binary alloys, providing unprecedented predictive fidelity across diverse compositional and structural spaces [68–70]. Furthermore, active learning frameworks have been developed to iteratively refine MLIPs on the fly during simulations, allowing the potential to adapt dynamically to evolving atomic environments. This capability is particularly critical for simulating non-equilibrium processes, defect formation, and surface/interface dynamics in alloys, where traditional fixed-form potentials often fail. The combination of MLIPs with high throughput simulations and multiscale modeling thus offers a powerful platform for the predictive design of advanced binary alloys with tailored mechanical, thermal, and electronic properties. Although MLIPs (e.g., MTP, GAP) achieve near DFT accuracy, generating high-quality training datasets remains a costly and highly skilled process, especially in the large structural and compositional spaces of binary alloys. Furthermore, the extrapolation capability of MLIPs beyond the training data space remains an ongoing research issue.

5.2.2. Digital twins of material lifecycles

The concept of digital twins virtual, high fidelity replicas that represent the entire lifecycle of materials from synthesis through service induced degradation is rapidly gaining traction in the field of alloy research. These platforms integrate multi-scale computational simulations, including DFT, MD, and Finite Element Methods (FEM), with experimental feedback derived from in situ characterization techniques such as electron microscopy, X-ray diffraction, and spectroscopy. By combining operational data streams from sensors and performance monitoring, digital twins provide a dynamic, continuously updated representation of material behavior under realistic conditions. In the context of binary alloys, digital twins offer the capability to track microstructural evolution, grain growth, phase transformations, defect nucleation, and accumulation over time, enabling predictive modeling of mechanical, thermal, and

chemical performance. Such models facilitate anticipatory maintenance, lifetime prediction, and real time optimization of components in demanding service environments, including aerospace engines, energy systems, and biomedical implants [71, 72]. By bridging atomistic simulations, mesoscale modeling, and experimental validation within a unified framework, digital twins represent a transformative paradigm for materials design, process control, and reliability assurance, accelerating the translation of computational insights into industrially deployable alloy solutions. Implementing a Digital Twin is not only challenging in terms of simulation but also in terms of data infrastructure and system integration. It requires continuous, real-time integration between multi-scale models (DFT, MD, FEM), experimental sensor data (in situ characterization), and industrial operational systems. Challenges of data compatibility, metadata standardization, and building automated feedback loops are the biggest barriers to implementing a Digital Twin in a real world production environment.

5.2.3. Quantum computing for electronic structure

Classical DFT approaches, while highly effective for many materials, are fundamentally constrained when addressing systems with strongly correlated electrons or large-scale quantum phenomena. These limitations hinder accurate modeling of electronic structure, magnetism, and excitonic effects in complex binary alloys. Quantum computing, leveraging algorithms such as quantum phase estimation and variational quantum eigensolvers (VQE), presents a promising pathway to surmount these challenges by enabling direct solutions of the electronic Schrödinger equation on quantum hardware. Although currently in its early developmental stages, quantum algorithms have already demonstrated successful simulations of small molecules and simplified Hubbard models, establishing proof-of-concept for future applications in materials science [73, 74]. Looking forward, quantum simulation holds the potential to revolutionize the prediction of electronic properties in complex binary systems, including band structures, magnetic ordering, and excitonic behavior in alloys such as Fe–Ni, MoS_2–WS_2, and other technologically relevant compounds. By enabling quantum-level accuracy for systems that are intractable with classical methods, quantum-enabled computational frameworks could unlock fundamentally new insights into alloy behavior, guiding the design of high performance materials for electronics, energy, and spintronic applications. The integration of quantum simulation with classical multiscale modeling and machine learning represents a forward looking strategy to expand the predictive reach of computational alloy design. Then they have to face the challenges of Quantum Computing because this field is still in the early developmental stages. Current algorithms can only successfully simulate small molecules or simple Hubbard models. Technical barriers such as high error rates of qubits, decoherence, and scalability issues for complex material systems (e.g., a large alloy crystal) are major challenges that will take decades to solve

5.3. Toward autonomous materials design

The convergence of artificial intelligence (AI) enhanced modeling, real-time experimental integration, and emerging quantum computing technologies is ushering in a transformative era of autonomous materials design. Within this paradigm, computational simulations evolve from passive predictive tools into active agents embedded in closed loop design systems, capable of generating hypotheses, guiding synthesis, validating experimental outcomes, and dynamically adapting to feedback. For binary alloys, such autonomous frameworks envision the rapid identification of compositions with tailored mechanical, electronic, thermal, or biocompatible properties; predictive modeling of microstructural evolution under realistic service conditions; and real-time optimization of processing parameters, all with minimal

human intervention. Initiatives such as the Materials Genome Initiative (MGI), AFLOW, and NOMAD provide the essential computational infrastructure, high fidelity datasets, and standardized descriptors required for training and deploying these intelligent design agents. Realizing this vision will necessitate close interdisciplinary collaboration among materials scientists, computational physicists, data engineers, and manufacturing specialists, fostering integration across simulation, characterization, and fabrication domains [75]. By combining AI, multiscale modeling, quantum-enabled simulations, and digital twin frameworks, the materials community can accelerate the discovery to deployment cycle for binary alloys, enabling a new generation of high performance, application specific materials and establishing a paradigm shift in how alloys are designed, optimized, and industrially implemented. Currently, many studies have linked the results of experimental methods with the results of simulation methods to compare, contrast and confirm each other's results and predictions, creating a rich database for comparison and sharing with the world community. In that, with the proposed recommendations:

-ML Experiment Integration: Develop closed-loop feedback systems where ML enhanced predictions are sent to automated synthesis and characterization systems (e.g., Robotic Labs) for validation and collection of new experimental data. This data is then used to refine the ML model, forming an autonomous materials design cycle.

-Develop Open Access Alloy Databases: Invest in building standardized repositories (using unified metadata) that contain not only DFT data but also multi-condition experimental data (elevated temperature properties, mechanical properties under load, heat treatment data, etc.). Initiatives such as AFLOWLIB and NOMAD need to be expanded to integrate experimental and simulation data from different scales (DFT, MD, FEM).

-Multiscale Modeling Enhancement: Priority is given to the development of hybrid approaches and multiscale modeling software that can automatically link accurate predictions from DFT (quantum level) with large-scale dynamics of MD and continuum level modeling (Phase Field, FEM), to solve complex microstructure and large deformation problems under realistic conditions (e.g., simulation of casting or 3D printing processes).

-MLIP Validation and Expansion: Research focuses on validating the transferability and extrapolation of Machine Learning Force Fields (MLIPs) for novel binary alloy systems and non-equilibrium conditions.

6. Conclusion

The convergence of computational simulation and materials science has catalyzed a transformative paradigm in the discovery, design, and optimization of binary alloys. Modern simulations now provide atomistic and quantum level insights, elucidating mechanisms such as dislocation nucleation, grain-boundary evolution, and phase stability, while simultaneously enabling predictive modeling of thermal, electronic, and mechanical properties. The case studies examined from Si–Ge semiconductors and MoS_2–WS_2 2D alloys to Ti–Nb biomedical and Al–Mg structural systems illustrate how theoretical predictions increasingly align with experimental validation, high-throughput synthesis, and industrial deployment. Despite these advances, several challenges persist. Force field limitations constrain the accuracy of molecular dynamics simulations, the computational cost of DFT and large-scale modeling restricts system size and timescales, and gaps remain in integrating multi-fidelity simulation data with real-world experimental workflows. Emerging strategies including machine learned interatomic potentials, digital twin platforms, and quantum computing offer robust pathways to overcome these bottlenecks, enabling high-fidelity, scalable, and adaptive simulation frameworks that closely mirror physical reality. Looking

forward, the future of binary alloy research lies in closed-loop, simulation-informed ecosystems capable of autonomously guiding synthesis, characterization, and deployment. By unifying AI enhanced modeling, multiscale simulation, and real-time experimental feedback within a coherent data centric framework, the materials community can accelerate innovation cycles, reduce development costs, and engineer alloys with unprecedented functional performance. The frontier is no longer defined by computational limitations; rather, it is shaped by the ability to integrate and orchestrate diverse predictive tools into a synergistic platform for next-generation materials discovery.

Funding: The work received no funding.

Data Availability Statement: The data that support the findings of this study are available from the corresponding author upon reasonable request.

Competing interests: The authors declare that they have no competing interests.

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