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TWO-DIMENSIONAL ZnO NANOSTRUCTURES: A COMPREHENSIVE REVIEW

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Abstract
Two-dimensional ZnO nanostructures are attractive for photocatalysis, sensors, and nanoelectronics because they have special mechanical, optical, and electrical characteristics that set them apart from bulk ZnO. The stability of planar honeycomb ZnO monolayers with a direct bandgap has been demonstrated by DFT research[1] whereas Zn-3d electron localization is improved by hybrid and DFT+U approaches[2]. Large-scale defect regulation and vacancy effects are addressed by classical MD simulations, which enhance these investigations. Additionally, recent research demonstrates vacancy-enhanced photocatalysis in ZnO nanosheets and strain-induced phase transitions in ZnO nanofilms.[3] The combination of classical and DFT simulations offers a thorough foundation for customizing 2D ZnO for device applications.

INTRODUCTION

1.1 Motivation for studying 2D ZnO

The interest in research on two-dimensional zinc oxide (2D ZnO) stems from the unique characteristics that make it different from ZnO. In the paper "Atomic Scale Study on Growth and Heteroepitaxy of ZnO Monolayer on Graphene (Hong et al., 2017)," the researchers experimentally demonstrate that the formation of graphene-like structures and quantum confinement enables a single-layered ZnO deposited on graphene to have a band gap as large as ~4.0 eV[4]. Similarly, theoretical ideas (e.g., "Doping in the two-dimensional limit: p/n-type defects in ML ZnO" by D. Han et al., 2022) investigate the differences between bulk behavior and the electronic structure in monolayer ZnO, particularly with regard to band edges and defect levels[5]. These increase the gap and provide new avenues for UV optoelectronic applications.

A further incentive is to adjust functioning through rare-earth substitution, adsorption, or doping. For instance, first-principles calculations in Al-Doped ZnO Monolayer as a Promising Transparent Conducting Electrode (Wu et al., 2017) show that Al doping in a ZnO monolayer enhances conductivity while preserving high optical transparency, which is crucial for transparent electrodes[6]. Furthermore, the incorporation of First Principles Pd in ZnO monolayers increases adsorption affinity towards gas molecules, thus increasing sensitivity, as mentioned in Insight into Pd-Doped ZnO Monolayers as a Gas Sensor. (Q. Zhou et al., 2020)[7].

Table 1. Motivation & Unique Properties of 2D ZnO

Property /Feature	Details	Relevance
Structural stability	Graphene-like (honeycomb) 2D ZnO stable at monolayer thickness before transforming to bulk wurtzite	Explains why ultrathin sheets form
Edge magnetism	Zigzag edges show localized ferromagnetic behavior; armchair edges are nonmagnetic	Potential in spintronic devices
Exciton binding energy	60 meV (bulk); even stronger in 2D due to confinement	UV optoelectronics & excitonic devices
Bandgap tunability	Thickness, strain, and edge configuration strongly affect electronic gap	Bandgap engineering for devices

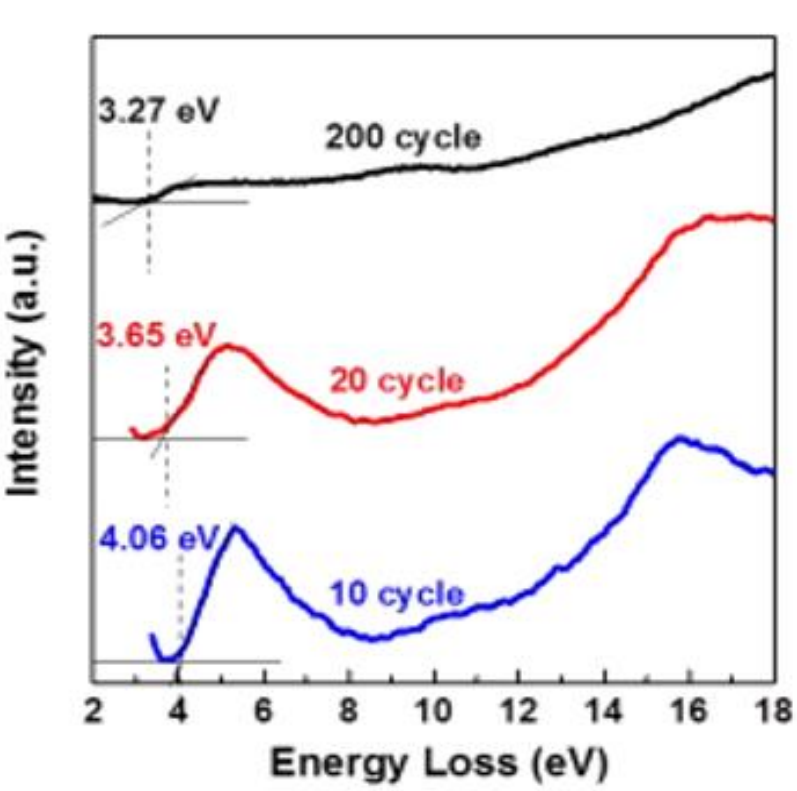

Fig. 1. STEM-EELS spectra of ZnO deposited with different ALD cycles on UV/ozone-treated graphene [10]

Moreover, physical and chemical reactivity of 2D ZnO surfaces can be beneficial in catalytic and sensing applications. The paper "Adsorption and evolution of N_2 molecules over ZnO monolayer: a combined DFT and kinetic Monte-Carlo insight" (Ghosh, Nath & Sanyal, 2024) studies the adsorption, diffusion, and evolution of N_2 molecules on the surface of the ZnO monolayer and shows how layer number, temperature, and pressure influence the surface coverage, adsorption energy, and diffusion barrier [8]. The paper "Epitaxial growth of ZnO films on Cu(111) surface" (Thang et al., 2019) also demonstrates problems associated with the stability of structural phase in the monolayer limit as it shows how ultrathin ZnO layer on copper surface changes its polymorphic structure from graphitic to wurtzite above certain thickness (~5 layers)[8].

1.2 Experimental progress on 2D ZnO synthesis

Epitaxial monolayer formation on 2D or metal surfaces is a significant experimental breakthrough. A ZnO monolayer was deposited atomically on graphene by Hong et al. (2017). They recorded optical transparency and band gap ≈4.0 eV for the thinnest layers, confirmed

structure with TEM, and tracked growth atom by atom, particularly at zigzag edges[4]. The optical and structural characterization is also described in Epitaxial Growth of ZnO Monolayer Film on Graphene: The Thinnest Metal Oxide (Hong, Lee, Kim, Son, et al., 2017)[9]. ng, Lee, Kim, Son, et al., 2017)[9].
Furthermore, there have been attempts to control thickness and phase using substrate support. According to the research titled "Epitaxial growth of ZnO films on Cu(111) surface" (Thang et al., 2019), the ZnO maintains its graphitic-like (planar) structure below roughly five layers, but above that it changes to the wurtzite structure. This aids in defining monolayer stability bounds[8].

Furthermore, functionalization and sensing approaches are growing. Adsorption of organic TCNQ on ZnO monolayer, for instance, was studied using density functional theory (Chen et al., 2024). The results indicate that adsorbing TCNQ (tetracyanoquinodimethane) on ZnO monolayer results in effective p-type doping and alters the band gap, which might be utilized in doping techniques[10]. Additionally, Pd-doped monolayers have been investigated experimentally and computationally to provide improved gas sensing capabilities for reactive or dangerous gases. One such instance is the first-principles study by Zhou et al. (2020) (ACS Omega)[7].

Table 2. Experimental Progress in 2D ZnO Synthesis

Method	Key Findings	Thickness / Shape Control
Surfactant-assisted ionic layer epitaxy (SA-ILE)	Air-water interface growth using surfactants (e.g., oleyl sulfate);parameter map for uniform nanosheets	Few nm, uniform sheets
Ionic layer epitaxy (ILE) with EDL confinement	Control of single-crystalline nanosheets at unit	1–4 unit cells
Post-annealing $Zn(OH)_2$	Converts $Zn(OH)_2$ nanosheets into ultrathin ZnO	Thickness ~1–3 nm
Hydrogel-assisted electrodeposition	Nanosheets, nanoflakes, and hierarchical structures grown on electrodes	Morphology tuned by deposition

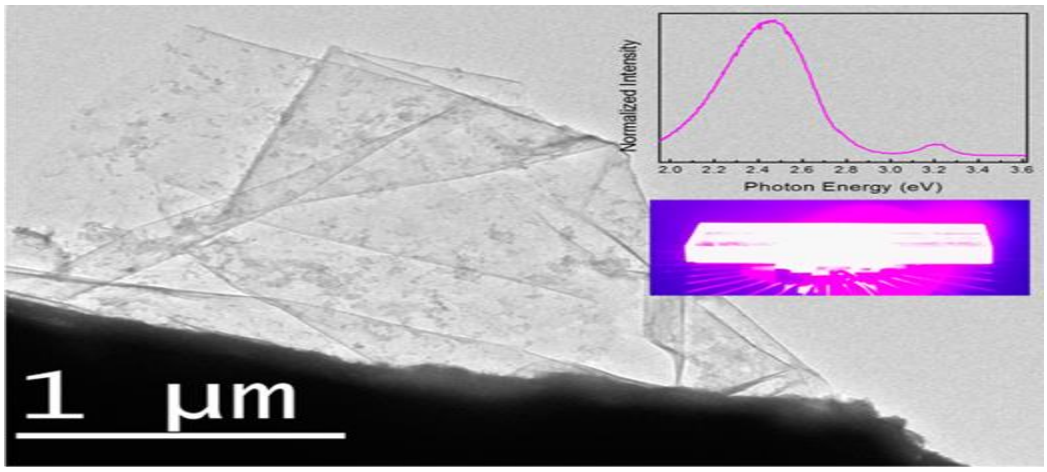

Fig. 2. The crisp, straight edges and transparency confirm the material is only a few atoms thick (a 2D material) [11]

1.3 Role of simulations in understanding 2D ZnO properties

For 2D ZnO, simulations offer vital information on defect energetics, doping, adsorption, etc. Formation energies, ionization levels, and stability of donor and acceptor defects in the monolayer limit are extensively calculated in the study "Doping in the two-dimensional limit: p/n-type defects in ML ZnO" (Han et al., 2022). This makes it easier to distinguish between

shallow and profound flaws, which is important for carrier engineering[5]. Similarly, high-accuracy predictions for oxygen and zinc vacancy levels using hybrid functionals are provided in Accurate Energy Level of Point Defects from Non-Empirical Screened Range Separated Hybrid Functional Theory: The Case of Zinc Oxide Vacancy (Ke, Gant, Kronik, Neaton, 2025). Methods and insights are directly applicable to 2D expansions, even if this is primarily for bulk ZnO[12].

Doping and functionalization are also covered in simulations: Al substitution in ZnO monolayer enhances optical and electronic conduction while maintaining transparency, as has been shown in Al-Doped ZnO Monolayer as a Promising Transparent Conducting Electrode (Wu et al., 2017)[6]. Initial Principles The 2020 study Insight into Pd-Doped ZnO Monolayers as a Gas Sensor examines how Pd doping alters the adsorption behavior (gas molecules, charge transfer) on ZnO monolayers and provides predictions that are helpful for sensor design[7]. Additionally, simulations aid in the comprehension of catalytic action and surface adsorption. N_2 molecule adsorption and evolution on ZnO monolayer surface: a theoretical DFT and kinetic Monte-Carlo study (Ghosh, Nath & Sanyal, 2024) models the effects of layer number on adsorption, the evolution of coverage with temperature and pressure, and the interactions of N_2 (adsorption energy, diffusion) with the monolayer. This type of research connects the atomic scale to the environment and real-world circumstances[13]. Additionally, Chen et al. (2024) demonstrate how organic molecules can modify electronic behavior by offering pathways for doping or functionalization in their Density Functional Theory Study of Adsorption of Organic TCNQ on ZnO Monolayer[10].

Table 3. Reported Band Gaps of ZnO (Bulk vs 2D)

MATERIAL / STRUCTURE	METHOD	REPORTED BAND GAP (EV)
BULK ZNO	Experiment	~3.3
2D ZNO MONOLAYER (PLANAR)	DFT (PBE)	~1.81
2D ZNO MONOLAYER	GW	~3.01
2D ZNO ULTRATHIN NANOSHEET	Experiment (optical)	up to ~4.0 (quantum confinement)

2. Structural Overview of 2D ZnO

Due to the tunable electrical, optical, and piezoelectric properties of the 2D ZnO, it has become a favorable wide-bandgap semiconductor. Ultrathin ZnO sheets take on different atomic-scale shapes in contrast to bulk ZnO, which crystallizes in a wurtzite structure. These structures' crystallographic arrangement, thickness, presence of defects or dopants, and responsiveness to strain all have a significant impact on their stability and usefulness. We list the main features of 2D ZnO structure below.

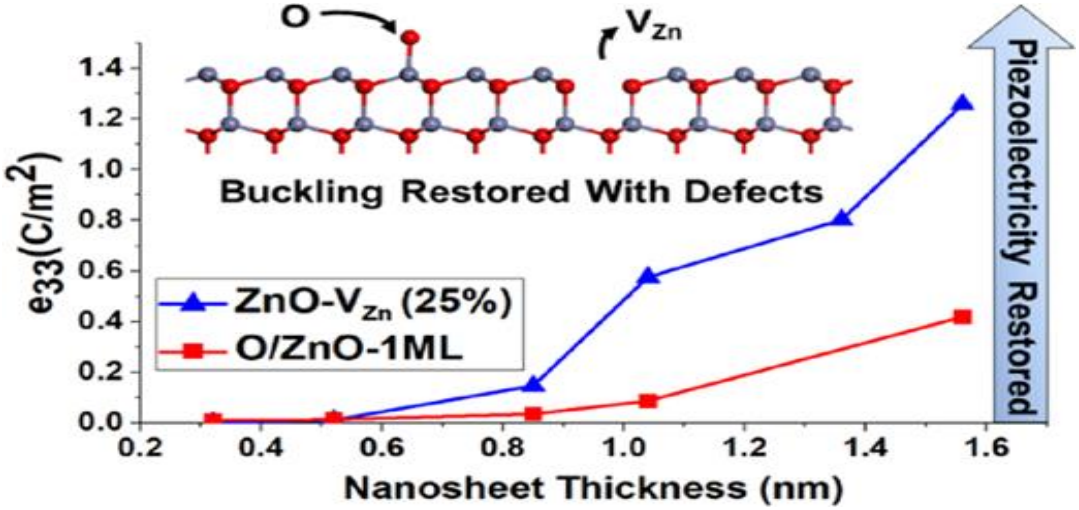

Fig. 3. Shows the restoration of piezoelectricity in zinc oxide (ZnO) nanosheets as their thickness increases, enhanced by defects such as zinc vacancies and oxygen adatoms (O)[14]

Using the density functional theory method, we show that a 1 ML surface coverage of oxygen and 25% concentration of zinc vacancies can bring back the buckling effect in few-layered 2D ZnO sheets. With a thickness of 1.48 nm and 25% Zn vacancy concentration, we can obtain an e33 value of 1.26 C/m2, which is a 120% enhancement over the bulk value. This approach has the ability to screen out the piezoelectric performance of other materials, and it shows that defects can be used to bring back the wurtzite phase and dielectric properties in ultrathin 2D ZnO sheets, thus making them applicable in nanoscale piezoelectric devices.

2.1 Crystallographic forms (planar vs buckled)

According to the early theoretical research, ZnO can create a planar honeycomb lattice that resembles graphene, with oxygen and zinc atoms occupying the same plane[1]. However, when isolated, dynamic instabilities in this flat structure were found using phonon dispersion simulations. In order to address this, a buckled ZnO sheet was suggested, in which the vertical displacement of Zn and O atoms produces polarity and improves structural stability[15]. The material is better suited for free-standing applications because of this buckling, which decreases symmetry while stabilizing vibrational modes.

Functionally, buckled ZnO demonstrates polarity and piezoelectricity, which makes it perfect for strain-tunable and nanogenerator applications, whereas flat ZnO has broader bandgaps and resembles a fully covalent system[14].

Table 4. Crystallographic Forms (Planar vs Buckled)

ORM	STRUCTURE FEATURES	STABILITY	FUNCTIONAL PROPERTIES
PLANAR ZNO	Honeycomb graphene-like lattice (Zn and O in same plane)	Dynamically unstable (phonon dispersion shows instabilities)	Wider bandgap, covalent bonding nature
BUCKLED ZNO	Zn and O atoms vertically displaced	Stable (suppresses vibrational instabilities)	Polarity, piezoelectricity → good for nanogenerators

2.2 Monolayer vs few-layer ZnO

The ultimate 2D limit is a monolayer ZnO, which is dominated by severe quantum confinement effects and surface states. This is advantageous for UV optoelectronics and gas sensors owing to its large direct band gap (>3.0 eV) and very high reactivity [1]. However, it

requires substrates or encapsulation due to its comparatively low free-standing stability.
Interlayer van der Waals and ionic interactions stabilize the nanosheets as the number of layers rises. The bandgap narrows in few-layer ZnO as a result of improved dielectric screening and less confinement[15]. Optoelectronic qualities can be adjusted thanks to this thickness dependence. Furthermore, tunable band alignment and defect control are provided by heterostructures of monolayer and few-layer ZnO with other 2D materials (such as MoS_2 and graphene), expanding applications in energy devices and catalysis[16].

Table 5. Monolayers vs Few-layer ZnO

TYPE	STABILITY	BANDGAP	APPLICATIONS
MONOLAYER	Low free-standing stability (needs substrate/encapsulation)	Wide direct bandgap >3.0 eV (strong confinement)	UV optoelectronics, gas sensing
FEW-LAYER	Higher (due to interlayer van der Waals/ionic interactions)	Narrower bandgap (screening reduces confinement)	Tunable optoelectronics, heterostructures for catalysis & energy

2.3 Defects and dopants in 2D ZnO

The properties of 2D ZnO are greatly affected by the intrinsic point defects like anti-sites, zinc vacancies (VZn) and oxygen vacancies. (V_o). Typically, oxygen vacancies introduce free electrons and change conductivity by acting as shallow donors. Their significant contribution to carrier production and even magnetism is confirmed by computational investigations.
Doping increases functionality even further. For example, non-metal doping (N, P, S) can permit p-type conductivity, which is otherwise challenging to produce in ZnO, whereas transition-metal doping (Fe, Mn, Co) causes magnetic moments for spintronics[16]. It's interesting to note that dopants and flaws work in concert to improve catalytic and sensing performance. For instance, Fe-doped ZnO with designed oxygen vacancies exhibits greater adsorption sensitivity, which makes it desirable for photocatalysis and gas sensors.

Table 6. Defects and Dopants in 2D ZnO

TYPE	EXAMPLE	EFFECT	APPLICATIONS
INTRINSIC DEFECTS	Oxygen vacancy (V_o)	Acts as shallow donor → increases conductivity, introduces magnetism	Gas sensing, photocatalysis
NON-METAL DOPANTS	N, P, S	Enables p-type conductivity (difficult in ZnO)	p–n junction devices
TRANSITION-METAL DOPANTS	Fe, Mn, Co	Induce magnetic moments	Spintronics

2.4 Mechanical stability and strain tuning

A crucial prerequisite for flexible 2D systems is mechanical stability. Molecular dynamics simulations and elastic constant analysis show that ZnO nanosheets are capable of withstanding moderate uniaxial and biaxial strain without collapsing. Ultrathin ZnO films showed resistance to mechanical deformation in experiments[17]. Crucially, the bandgap is directly tuned by strain. In general, compressive strain raises the bandgap while tensile strain decreases it. Biaxial strain and bandgap have been found to have a nearly linear relationship, which presents opportunities for strain-engineered optoelectronics[18]. Additionally, strain improves piezoelectric characteristics,

opening up energy harvesting applications. It has been demonstrated that piezoelectric polarization in monolayer ZnO can be restored or enhanced via defect-assisted strain engineering[14].

Table:7. Mechanical Stability and Strain Tuning

PROPERTY	BEHAVIOR UNDER STRAIN	APPLICATION
ELASTIC STABILITY	Can withstand moderate uniaxial/biaxial strain without collapse	Flexible electronics
BANDGAP TUNING	Compressive strain ↑ bandgap, tensile strain ↓ bandgap (linear relation)	Strain-engineered optoelectronics
PIEZOELECTRIC RESPONSE	Enhanced under strain, defect-assisted strain engineering boosts effect	Energy harvesting

3. Classical Simulations of 2D ZnO

3.1 Overview of classical methods (MD, MC, force fields)

A computationally effective method for investigating the structural and dynamic characteristics of 2D ZnO is using classical simulations. The most popular approach among these is called Molecular Dynamics (MD), that employs the equations of motion developed by Newton in studying atomic motions at low temperatures.MD has been widely used to investigate ZnO nanosheet stability, flaws, and strain effects[19]. In addition to MD, Monte Carlo (MC) simulations use stochastic sampling to study equilibrium properties, specifically adsorption energetics and defect thermodynamics.

The foundation of classical simulations is force-field-based methods, which enable scale modeling of systems with tens of thousands of atoms. Classical approaches shed light on mesoscale processes like fracture, grain boundary diffusion, and large-scale phonon transport, in contrast to ab initio techniques, which are restricted to a few hundred atoms. To capture the ionic-covalent bonding feature of ZnO, many-body force fields and pairwise potentials have been constructed.

The usefulness of MD and MC is further increased by its interaction with multiscale modeling frameworks. For instance, MD can supply temperature-dependent elastic constants that can be used as inputs in ZnO nanomembrane continuum-level models. Hybrid methods also make it possible to connect large-scale atomic dynamics with electronic-level data (via DFT). Because of this, in 2D ZnO research, classical simulations are essential for bridging length and time scales.

Table 8: Classical Methods for 2D ZnO (MD, MC, Force Fields)

METHOD	WORKING PRINCIPLE	APPLICATIONS IN ZNO	STRENGTHS	LIMITATIONS
MOLECULAR DYNAMICS (MD)	Solves Newton's equations of motion to track atomic trajectories	Stability of nanosheets, defects, strain effects, phonon transport	Captures dynamics, temperature effects	Limited by potential accuracy, short time scales (ns–μs)
MONTE CARLO (MC)	Uses stochastic sampling of configurations	Adsorption energetics, defect thermodynamics, equilibrium properties	Efficient for thermodynamic averages	No dynamics, depends on good sampling
FORCE FIELDS (FFS)	Approximate atomic interactions	Large-scale modeling (fracture, grain	Scales to 10^4–10^6 atoms	Accuracy depends on potential choice

	with parameterized potentials	boundaries, diffusion)

3.2 Interatomic potentials for ZnO (Buckingham, ReaxFF, Tersoff)

The Buckingham potential, which combines long-range Coulomb interactions with short-range exponential repulsion and van der Waals (dispersion) attraction, is still the preferred interatomic model for simulating ionic activity in 2D and nanostructured ZnO systems. Mechanical properties of size dependent ultrathin ZnO nanowires have been successfully predicted by studies using Buckingham potentials.

For example, "Structure-dependent mechanical properties of ultrathin zinc oxide nanowires" states that the yield strength and Young's modulus of zinc oxide nanowires increase when the diameter reduces.. The Buckingham form plus Coulombic terms capture deformation behaviors and phase transformations (between wurtzite and hexagonal-like structures)[20].

Reactive Force Fields (ReaxFF) have been parameterized especially for ZnO to examine dynamic phenomena like oxidation, surface annealing, and defect evolution in order to capture bond creation and breaking in nanostructures. . For example, in the paper entitled "A Reactive Force Field (ReaxFF) for Zinc Oxide," Raymond, van Duin, Baudin, and Hermansson (2008) discuss how they fitted to a training set of quantum mechanical data like surfaces, energies, geometries, and charge densities to produce a ReaxFF parameterization of ZnO .With strong agreement to DFT and experimental results, this potential has been utilized to simulate structural changes of ZnO under a variety of circumstances[21].

Table 9: Interatomic Potentials for ZnO

POTENTIAL TYPE	FUNCTIONAL FORM	APPLICATION IN ZNO	KEY FINDINGS
BUCKINGHAM + COULOMB	Short-range repulsion + long-range electrostatics + vdW attraction	Nanowires, nanosheets, bulk phases	Size-dependent mechanical properties (↑ modulus & yield strength with ↓ diameter)
REAXFF	Bond-order potential, allows bond breaking/formation	Oxidation, surface annealing, defect evolution	Captures chemical reactions, matches DFT for ZnO
TERSOFF-LIKE POTENTIALS	Angular-dependent, many-body covalent interactions	ZnO surfaces, mechanical response under strain	Captures directional bonding effects; less common for ionic ZnO

3.3 Applications of MD in 2D ZnO

- **3.3.1 Thermal and mechanical stability**

For purposes of examining the thermal stability of ZnO monolayers and nanoribbons, MD simulations have been used extensively. Planar ZnO is metastable at room temperature, according to both ab initio and conventional MD, but buckled structures maintain stability at higher temperatures[1].

Additionally, mechanical stability under compressive and tensile strain has been investigated. ZnO nanosheets are highly flexible up to about 6–8% strain before breaking, according to classical MD. Extracted stress-strain curves from MD correspond well with the outcomes of the experimental AFM nanoindentation

The mechanical reaction is considerably altered by the addition of flaws and dopants. According to MD investigations, dopants like magnesium or aluminum can strengthen the lattice against fracture, however oxygen vacancies lower tensile strength. This demonstrates how MD may be used to forecast the creation of mechanically resilient 2D ZnO materials

- **3.3.2 Surface reconstructions and edge effects**

Surface reconstructions and edge states are very important because of 2D ZnO's large surface-to-volume ratio. This dynamic reconstruction of surface atoms can lead to different surfaces, like Zn-terminated and O-terminated edges,which significantly affect stability and polarity, is captured by MD simulations[22].

Simulations of surface chemistry under environmental variables are made possible using classical potentials, especially ReaxFF. For instance, hydroxylated surfaces and edge site rebuilding result from the adsorption of H_2O and O_2 molecules. ZnO-based sensors' experimental observations are explained by these calculations.

Additionally, localized electronic states that impact optical response are introduced by edge-specific reconstructions. According to MD research and tight-binding models, armchair edges stay nonmagnetic while zigzag edges tend to sustain ferromagnetism[1].

- **3.3.3 Phonon and heat transport**

The lifetimes of particular phonon modes are also revealed by spectral energy density (SED) analysis in MD. According to these findings, optical phonons contribute more to heat transmission in ZnO monolayers than in bulk, where acoustic phonons predominate.

Phonon transport is drastically changed by strain engineering. According to MD simulations, compressive strain stiffens the lattice, enhancing heat transmission, while tensile strain softens acoustic phonon modes, reducing thermal conductivity. These results provide credence to the usage of ZnO in thermoelectric applications[18].

3.4 Limitations of classical methods for ZnO

Classical approaches have transferability problems notwithstanding their benefits. Buckingham and ReaxFF are examples of interatomic potentials that are parameterized for particular phases and might not apply to surfaces, defects, or heterostructures. This reduces the precision of forecasting novel configurations that were left out of the parameter fitting process.

The absence of specific electronic structural knowledge is another drawback. Charge transfer, excitonic effects, and defect-induced localized states—all essential for optoelectronic applications—cannot be captured by classical MD. To bridge this gap, hybrid strategies like quantum–classical embedding are being developed.

Lastly, trade-offs between accuracy and computing cost are still difficult to resolve. MD is capable of simulating nanosecond dynamics for large systems, but it is unable to reach the microsecond or millisecond timescales that are important for long-term stability and diffusions[23].

4. DFT Simulations of 2D ZnO

4.1 Fundamentals of DFT and exchange-correlation functionals

Density Functional Theory (DFT) is the widely applied quantum mechanical technique used for analyzing the electrical, structural, and optical properties of 2D ZnO. The ground state properties can be analyzed computationally by using the DFT technique, which involves the reduction of many-body Schrodinger equation to that of one-body Kohn-Sham equation. The exchange correlation (XC) functional plays an important role in the accuracy of the predictions made through it. Some common XC functionals include Generalized Gradient Approximation (GGA) and Local Density Approximation (LDA)significantly underestimate the bandgap of ZnO while frequently producing acceptable lattice constants[24].

Better bandgap predictions are offered by hybrid functionals, such HSE06, which integrate precise Hartree-Fock exchange. In considerably better agreement with measured UV absorption values, PBE-GGA estimates gaps for ZnO monolayers, whereas the HSE06 and GW approximations yield gaps . ZnO is also subjected to many-body techniques , in order to investigate excitonic effects, which are more noticeable in 2D materials because of decreased screening[25]. Predictions for strain response, dielectric behavior, and defect energetics are likewise impacted by the selection of the XC functional. ZnO monolayers have a direct bandgap and a stable honeycomb structure that may be adjusted by biaxial strain, as shown by Behera & Mukhopadhyay (2011). ZnO's function in UV optoelectronics is further supported by hybrid functionals, which further validate the durability of direct transitions. Reliable defect modeling

and heterostructure design are ensured by appropriate functional selection[26, 27].

4.2 Structural optimization and electronic band structure

Optimized 2D ZnO structures using DFT reveal a planar honeycomb lattice with Zn–O bond lengths ~1.9 Å and lattice constant ~3.28 Å. Van der Waals adjustments (DFT-D2/D3, optB86b-vdW) are required for few-layer ZnO in order to capture interlayer coupling[1]. proved the stability of ZnO monolayers and how they change with thickness. verified this using theoretical forecasts in line with nanosheet testing.

The band structure shows that ZnO monolayers are direct gap semiconductors at the Γ point.with O-2p orbitals dominating the valence bands and Zn-4s orbitals dominating the conduction bands. HSE06 (~2.6 eV) and GW (~3.3 eV) are closer to experimental UV absorption measurements, whereas PBE underestimates the gap (~1.7 eV)

According to research by Navarra et al., this tunability enables ZnO to be engineered for UV optoelectronic uses such as flexible photodetectors and transparent electrodes[28].

4.3 Optical and dielectric properties

The choice of exchange-correlation treatment is particularly important for ZnO because conventional LDA/GGA calculations suffer from a band-gap problem, which can introduce significant uncertainties in defect-level positions and defect formation energies. Lany and Zunger systematically assessed band-gap correction methods and finite-size effects for oxygen vacancies in ZnO **[29].**

Exciton confinement is influenced by the anisotropic dielectric response, wherein in-plane dielectric constants are greater than out-of-plane values. Ozgur et al.'s experimental ellipsometry investigations reinforce DFT predictions by confirming this anisotropy[30, 31]. The performance of thin-film devices depends on such direction-dependent dielectric effects.

4.4 Defect formation energies and electronic states

DFT is widely used to study intrinsic flaws like zinc vacancies (VZn) and oxygen vacancies (VO). VZn produces deep acceptor levels, whereas VO defects function as shallow donors, as shown by Janotti & Van de Walle[2]. Formation energies are considerably shifted by growth circumstances (Zn-rich vs. O-rich).

VO defects in 2D ZnO cause localized in-gap states and bandgap reduction, which is in line with experimental photoluminescence in thin ZnO films. Additionally, hydrogen interstitials serve as donors, which explains why ZnO nanostructures exhibit inadvertent n-type conductivity[29]. Kohan et al. studied the native point defects in zinc oxide (ZnO) using first principles calculations such as vacancies, interstitials, antistites, among others, with various charge states. [32].

4.5 Strain and external field effects

Biaxial strain alters the Zn-O bond length, and thus affects the electronic behavior of the ZnO monolayer. Behera and Mukhopadhyay have reported that the direct bandgap of graphene-like ZnO monolayer can be effectively engineered through biaxial strain., while the band gap remains direct within their investigated strain range of ±10%. The calculated nonlinear strain dependence demonstrates the potential of mechanical strain for band-structure engineering in 2D ZnO. [33, 34].

Stark shifts are caused by external electric fields, which lower bandgaps and increase optical absorption. In line with DFT trends in 2D ZnO, Makino et al. experimentally verified field effects in ZnO thin films.

Device applications are made possible by combined strain–field tuning. For instance, Tu et al. hypothesized that strain modifies ZnO heterostructures' band alignment, enhancing the efficiency of charge separation in photocatalysis and photovoltaics.

4.6 Heterostructures and interface simulations

Some recent studies on first principles show that 2D ZnO/MoS_2 heterostructures show type-II band alignment which helps in the ultra-fast separation of photogenerated carriers.. Ma et al. reported an HSE06 band gap of 1.59 eV for the ZnO/MoS_2 heterostructure and showed that photoexcited electrons and holes undergo rapid interlayer transfer. They further demonstrated that defects strongly regulate the carrier dynamics: oxygen vacancies in ZnO enhance

hole transfer, whereas sulfur vacancies in MoS_2 introduce defect states that promote electron–hole recombination."[35]
Another example is the 2D ZnO/SiC van der Waals heterobilayer, which has been investigated using first-principles DFT calculations. The stable stacking configuration has been found, and the heterobilayer shows high absorption coefficient, which is about cm^{-1}. The biaxial strain proves to be quite efficient to tailor the electronic and optical properties of Mo_2TiSe_5/Mo_3S_2, where the bandgap energy changes from 3.18 eV in −6% compression to 2.52 eV in +6% tension for pattern-I. It has been shown that strain engineering of heterostructures allows for the tailoring of the bandgap energy. and optical response of ZnO/SiC heterobilayers. [36].
MoS_2/ZnO and WS_2/ZnO heterostructures both display type-II band offset with significant conduction and valence band offsets, as well as enhanced optical absorption in visible-IR regions, which makes them perfect for photocatalysis and optoelectronic applications, according to the article "Electronic and Optical Properties of Heterostructures Based on MoS_2/ZnO and WS_2/ZnO [37]."

4.7 Comparison with experimental data
"The wurtzite ZnO lattice parameters reported experimentally by X-ray diffraction are approximately Å and Å, in reasonable agreement with calculated values. The review also reports an experimental ZnO band gap of approximately 3.3 eV."[30].
The dielectric constants (˜8.5) are in agreement with ellipsometry, and optical spectra from GW+BSE simulations match photoluminescence peaks. This confirms the optoelectronic performance predictions of DFT. Predicting the defect amount is still more difficult. Deep trap energies are underestimated by standard PBE; however, accuracy is increased by hybrid and GW approaches. Lany & Zunger [29]showed how advanced methods bring theory in line with experiment, highlighting the need for beyond-DFT corrections.

5. Case Studies

5.1 DFT study of planar vs buckled ZnO monolayers
DFT calculations (using both PBEsol and HSE06 functionals) are performed in the recent first-principles work "Novel ZnO nanosheet with buckling stress: First principles study" by Abdullah et al. (2024), which demonstrates that the band gap decreases as buckling increases in ZnO monolayers. Additionally, they verify that buckled ZnO monolayers maintain their thermal by investigating static and dynamic stability up to specific buckling heights with the aid of phonon spectrum and AIMD. [38].
"Using first-principles calculations, Chen et al. (2024) have studied the impact of planar buckling on the structural, electronic, optical, and photocatalytic properties of monolayer ZnO. It is shown that the increase of buckling height decreases the bandgap and shifts the band edge positions; adequate buckling provides good performance in visible light optical and water splitting photocatalysis." [39].
Additionally, "Chemical functionalization of the ZnO monolayer: structural" is the functionalization investigation. Adding H or F atoms (or mixed functionalization) raises buckling height, alters bonding (Zn–O–Zn angles), and causes a shift from planar to more buckled geometries. These changes have an impact on band structure, and depending on functionalization, both direct and indirect gaps appear (L. Chen, 2019)[39].

5.2 Classical MD of large-scale ZnO nanosheets
Kilic and Erkoç (2016) studied the structural behavior of pristine and defective ZnO nanosheets through classical molecular dynamics simulations. Defects such as vacancies, exchange, Stone-Wales like, line, and ring-like defects have been considered, and biaxial strain has been imposed along x- and y-directions at 1 and 300 K. "It has been shown from the results of the simulations that the structural behavior of ZnO nanosheets under biaxial strain depends on temperature, type of defect, boundary conditions, and strain rate." [40].
"Aghdasi et al. (2024) performed DFT calculations to explore the structural and elastic/plastic properties of ZnO monolayers doped with C, F, and P using 2×2 and 3×3 supercells". They found that doping generally

reduces the elastic and bulk moduli, with P doping producing the largest reduction. The yield strain also decreases under tensile loading for most doped structures, particularly under biaxial tension, demonstrating that chemical doping can substantially modify the mechanical stiffness and plastic response of ZnO nanosheets."[41].

5.3 DFT+U calculations for Zn 3d electrons

The localization and energetic position of these 3d electrons are often underestimated by standard DFT, particularly GGA, because ZnO contains Zn with a filled 3d shell. In order to enhance the description of localized states, DFT+U applies a Hubbard U correction. This leads to a more realistic hybridization between Zn-3d and O-2p orbitals, better band gap values (particularly in defect-rich structures), and better comparison with photoemission measurements. For example, Janotti & Van de Walle (Phys. Rev. B, 2007) demonstrated that usage of U leads to better band structure predictions of ZnO because it pushes Zn-3d orbitals into deeper states. [2].

"Volnianska et al. (2023) applied DFT calculations to study the influence of strain and near-surface environment on acceptor complexes in ZnO. The researchers showed that the effect of strain, especially compressive strain, and the near-surface environment could strongly affect the energy of formation of Zn vacancies and hydrogen-related acceptor complexes. "These findings give theoretical support to the experimentally observed dependence of acceptor-induced photoluminescence and p-type conductivity on the crystallography and dimensions of ZnO films and nanostructures."[42].

5.4 ZnO nanosheets with high vacancy concentrations

"Both computational and experimental studies demonstrate that oxygen-vacancy concentration strongly influences the functional properties of ZnO nanosheets. Yuan et al. showed that oxygen-vacancy-rich ZnO nanosheets exhibit enhanced sensitivity and faster response toward trace gases, which was attributed to defect-induced electronic-structure modification and increased surface activity. Similarly, Kochnev et al. (2023) combined experimental characterization and DFT computations for the study of ZnO nanosheets with varying concentrations of oxygen vacancies and other defects, proving that the concentration of defects affects the electronic configuration and photoluminescence of the nanosheets..[43].Similarly, Shen et al. (Chemosensors, 2023) showed that Zn and O vacancies modify adsorption energetics of harmful gas molecules, improving ZnO's sensing ability[3].

""Morales-Salvador et al. (2025) employed density functional theory calculations to study the effects of strain and thickness on the structural stability of ZnO nanofilms. It was found that biaxial strain could lead to structural phase transitions between BCT-ZnO and graphite-like ZnO phases, with the transition strain depending strongly on the thickness of the nanofilm." [44]. "Morales-Salvador et al. (2025) demonstrated that strain, nanofilm thickness, and strain-induced structural phase transformations can substantially alter the electronic characteristics of ZnO nanofilms, including the band gap and band-edge character, highlighting the importance of considering nanoscale structural effects when evaluating ZnO for applications such as photocatalysis, optoelectronics, and sensing."[49]

5.5 ZnO under tensile and compressive strain

The structural, optical, and catalytic performance of ZnO nanosheets is significantly impacted by vacancies, especially oxygen vacancies. Their effect is concentrated at low concentrations, resulting in shallow donor levels. On the other hand, vacancy-vacancy interactions at larger concentrations result in midgap states, defect bands, or in extreme situations, metallic conduction. Yuan et al. (Adv. Mater. Interfaces, 2019) showed that because of their narrower band gaps, vacancy-rich ZnO nanosheets had improved conductivity and photocatalytic activity.

Experimental and computational studies confirm the strong role of vacancy density. Yuan et al.'s work shows that vacancy-rich nanosheets serve as efficient gas sensors due to enhanced charge carrier availability. Complementary DFT studies, such as Kochnev et al. (Appl. Surf. Sci., 2023), reveal how varying oxygen vacancy concentrations modify photoluminescence,

band alignment, and optical absorption properties[43] .Similarly, Shen et al. (Chemosensors, 2023) showed that Zn and O vacancies alter adsorption energetics of toxic gas molecules, enhancing ZnO's sensing ability[3] .
The failure behavior and mechanical stability are also impacted by high vacancy concentrations. According to ab initio molecular dynamics and MD simulations of ZnO nanosheets with defects (e.g., Morales-Salvador et al., Nanoscale, 2025), vacancy accumulation causes local lattice distortions, decreases fracture strength, and speeds up crack propagation under strain [44]. These findings demonstrate that in order to accurately predict performance in photocatalysis, sensing, and nanoelectronics, genuine ZnO nanosheets—which infrequently maintain complete crystallinity—must be examined in vacancy-rich environments.

6. Multiscale Modeling Approaches

6.1 Coupling classical and quantum methods

"Multiscale modeling of ZnO can be improved with the use of quantum-mechanical and atomistic classical approaches. DFT allows us to have detailed data about electronic and atomic properties, while classical molecular dynamics makes it possible to simulate large systems and long timescales. In this case, Raymand et al. (2008) developed ReaxFF potential for ZnO using quantum-mechanical data, which include energy, geometry, and charge for Zn, ZnO bulk, low-index ZnO surfaces, and zinc hydroxide clusters. This ReaxFF model agreed well with DFT data on bulk and surface systems and was later used for MD simulations of vibrations and growth of ZnO bulk and surfaces."[45, 46].
"Multiscale approaches can bridge the accuracy of DFT with the larger spatial and temporal scales accessible through classical molecular dynamics. For $Zn_{1-x}Mg_xO$, Sepehrinezhad et al. (2024) used DFT data to develop a ReaxFF potential, which was subsequently employed to investigate composition-dependent ferroelectric properties and polarization switching at larger scales. [47].

6.2 Workflow for large-to-small scale modeling

Higher-level models are informed by the basic data these computations offer. Such first-principles investigations provide insight into the stability of intrinsic defects (zinc interstitials, oxygen vacancies) in ZnO and how they affect conductivity or catalytic activity[48].
After obtaining QM data, classical or reactive force fields are parameterized using it. Bond breaking, defect migration, and nanostructure stability spanning nanoseconds and tens of thousands of atoms are simulated for ZnO using ReaxFF and COMB3 potentials trained on DFT data. Research on ZnO nanowire breakage and defect dissemination shows how QM-trained potentials can exhibit large-scale behavior.
The process culminates with the incorporation of atomistic data into continuum or mesoscale models .In a ZnO nanoparticle development research, hollow and rod-like morphologies observed experimentally were successfully predicted by parameterizing a reaction-diffusion model using DFT kinetics[49].

6.3 Examples: Reactive simulations + DFT refinement

For instance, in ZnO surface reactivity studies, Raymand et al.'s ReaxFF ZnO model is commonly used to predict defect chemistry and adsorption, while DFT is applied later for fine electronic corrections. Reactive MD predicts adsorption configurations and bond rearrangements, while DFT refinement computes accurate energetics[45].
The production of ZnO nanoparticles is another example. In order to represent pattern creation, Báez et al. integrated a reaction–diffusion model with DFT-calculated reaction rates of precursor decomposition. The hollow and rod-like ZnO morphologies shown in experiments were replicated by their multiscale simulation[49, 50]. This demonstrates how QM+classical hybrid procedures can forecast novel morphologies in addition to explaining current behavior.
Multiscale refinement is essential in photocatalysis. In a study on ZnO photocatalysts, DFT refinement of charge transfer pathways was combined with reactive MD simulations (solvent, surface hydroxylation). The combined method demonstrated that photocatalytic efficiency is substantially modulated by surface termination and shape. [55 ,56]

6.4 Challenges in multiscale modeling of ZnO

The trade-off between accuracy and scalability is a significant obstacle. While force fields scale but

frequently misrepresent flaws and polar surfaces, DFT is precise but costly. Standard DFT functionals for ZnO require modifications (DFT+U, hybrid functionals, or GW) because they misplace Zn 3d levels and underestimate band gaps. Diffusion Monte Carlo (DMC) provides more accurate defect energetics than DFT, according to a comparative research, but system size is constrained by its cost[48].

Capturing flaws and environmental complexity is a second difficulty. The reactivity of ZnO is dependent on oxygen, water, or other adsorbates, and it displays a variety of polymorphs, surfaces, and defect chemistries. Reactive potential modeling necessitates a large amount of QM training data, and transferability is still restricted. As an illustration, ZnO's COMB3 and ReaxFF potentials frequently fall short of reproducing charge redistribution at defect locations.

Lastly, there are issues with validation and scale bridging. Spatial scales (microns) surpass atomistic models, and timescales pertinent to ZnO catalysis (milliseconds to seconds) are well beyond MD. Although they fill the gap, techniques like phase-field and kMC rely on precise input data. Furthermore, predictions are left dubious since validation against tests (such as defect spectroscopy and photocatalytic efficiency) is frequently lacking[51, 52].

Table: 9. Multiscale Modeling Approaches for ZnO

METHOD	SCALE	ADVANTAGES	LIMITATIONS
DFT (GGA, HYBRID, DFT+U, GW)	Electronic / Ångström (10^{-10} m); fs–ps	Accurate defect formation energies, adsorption, electronic structure	High computational cost, band gap underestimation (standard DFT), limited size/time
QUANTUM MONTE CARLO (DMC, VMC)	Electronic scale; fs–ps	Very high accuracy for defect energetics and band gaps	Extremely expensive; only small systems
REACTIVE FORCE FIELDS (REAXFF, COMB3)	Atomistic / nm; ps–ns	Bond breaking/forming, reactive simulations, large systems (10^5 atoms)	Needs careful parameterization, limited transferability, less accurate for defects
CLASSICAL FORCE FIELDS (BUCKINGHAM, LENNARD-JONES	Atomistic / nm; ps–ns	Cheap, scalable, good for bulk ZnO mechanical/thermal	Cannot capture reactivity or defect chemistry
MOLECULAR DYNAMICS (CLASSICAL OR REACTIVE)	nm–100s nm; ps–μs	Dynamic behavior, temperature effects, surface processes	Limited to short timescales; depends on force field accuracy
KINETIC MONTE CARLO (KMC)	nm–μm; μs–s	Accesses long timescales, defect diffusion, catalysis kinetics	Needs accurate input barriers (from DFT/MD); simplified dynamics
PHASE-FIELD MODELS	μm–mm; ms–s	Predicts morphology evolution (nanorods, hollow spheres, etc.)	Requires input from atomistic models; limited detail
REACTION–DIFFUSION MODELS	μm–mm; ms–s	Captures large-scale synthesis pathways, pattern formation	Simplified chemistry, depends on QM inputs

7. Current Challenges and Future Directions

7.1 Force field development for 2D ZnO

Why it's needed. The bonding, surface polarization, and reconstruction behaviors of two-dimensional and ultrathin ZnO (graphene-like or few-layer ZnO) are different from those of bulk wurtzite ZnO; these effects are frequently not reproduced by conventional force fields parameterized for bulk. Therefore, before any predictive large-scale MD of 2D ZnO can be relied upon, force fields that accurately capture changing charge/polarization, surface relaxations, and bond-breaking/forming for 2D motifs must be developed. See ZnO ReaxFF parameter efforts and general ReaxFF debates[48].

Approaches and progress. Reactive potentials (ReaxFF, COMB) or classical potentials are typically trained using the following workflows: (a) use DFT/hybrid functionals to compute a QM training set (surface energies, adsorption, defect structures), (b) optimize potential parameters to replicate those observables, and (c) validate on properties not used in training (phonons, surface reconstructions, defect migration). The above pipeline is illustrated through recent ab-initio based force fields development for ZnO, which also reveals that it may generate transferable potentials for aqueous/biomolecular settings[53].

Open challenges for 2D ZnO For 2D ZnO, important challenges include developing training sets that adequately describe charge redistribution, low-dimensional structural reconstructions, surface termination effects, and long-range electrostatic interactions. Transferability across different ZnO structures and environments also requires careful validation against high-accuracy quantum-mechanical calculations. Recent automated approaches such as JAX-ReaxFF and gradient-based optimization can accelerate force-field development by efficiently fitting reactive potentials to quantum-mechanical training data.. [54].

7.2 Accurate prediction of bandgap and excitonic effects

The problem. In low-dimensional ZnO or quantum-confined structures, excitonic binding energies (electron–hole interactions) and optical spectra necessitate techniques beyond simple DFT, , in order to obtain accurate optical predictions. Refer to research contrasting DFT+U and hybrid/GW/BSE methods for ZnO and graphene-like ZnO Franke et al. investigated mercaptocarboxylic-acid-functionalized ZnO(10-10) surfaces using both semilocal and hybrid density-functional calculations. The outcomes revealed that adsorption may create optically active states inside the band gap of ZnO, whereas calculations of the dielectric function using the PBE0 and TD-PBE0 levels demonstrated the resulting optical response of the hybrid ZnO–molecule system [55].

What works in practice. Beyond semilocal DFT, hybrid-functional and many-body approaches provide improved descriptions of the Optical and electronic characteristics of ZnO. Zhang and Schleife (2018) compared DFT, HSE06, G_0W_0, and self-consistent GW calculation for BN-ZnO and wurtzite ZnO and demonstrated substantial corrections to the underestimated DFT band gaps. They further employed the Bethe–Salpeter equation to calculate optical absorption spectra and exciton binding energies, explicitly accounting for electron–hole interactions. These results demonstrate the importance of quasiparticle and excitonic corrections for accurately describing the optical response of ZnO polymorphs." [56].

Practical tradeoffs & recommendations. Pawar et al. combined experimental characterization of ZnO thin films with First Principles Hybrid Functional Calculations to Study Film Thickness effects and orientation on quantum confinement and the electronic band gap. Their results showed that reducing the ZnO film thickness can substantially increase the band gap, with the quantum-confinement effect being stronger for the (100) orientation than for the (001) orientation." (PL, absorption, EELS)[57].

7.3 Defect engineering and doping at nanoscale

Importance and effects. The electrical, optical and photocatalytic characteristics of ZnO may be altered through the use of various defects, such as oxygen and zinc vacancies. Gurylev and Perng (2021) reviewed various approaches for synthesizing oxygen- and zinc-deficient ZnO and showed that controlled defect introduction can modify the electronic structure, charge-carrier transport, optical absorption, and photocatalytic behavior. These findings demonstrate the

potential of defect engineering for tailoring ZnO properties for specific applications." [58].

Modeling strategies. At the nanoscale, hybrid DFT (or DFT+U) and occasionally GW/DMC for benchmarking are necessary for precise prediction of defect formation energies, charge states, and diffusion pathways. In order to forecast dopant/defect distributions throughout growth or after treatment, multiscale procedures subsequently translate these QM energetics into kMC or continuum models. Numerous combined experimental and theoretical investigations demonstrate how defect populations in nanoparticles and thin films are regulated by synthesis conditions guided by DFT[49].

Challenges and research directions. An important challenge is achieving controlled dopant incorporation while understanding its influence on defect populations and optical properties at the nanoscale. Zhu et al. (2016) showed that Ga concentration and synthesis conditions strongly affect defect-related luminescence in ZnO nanoparticles, demonstrating the sensitivity of defect populations to processing conditions. Their cathodoluminescence analysis further showed that excessive Ga incorporation can generate negatively charged Zn vacancies and oxygen interstitials. [59].

7.4 Machine learning for ZnO potential development

Why ML potentials. "Machine-learning interatomic potentials (ML-IAPs) provide a route to large-scale atomistic simulations while retaining near-DFT accuracy. Zuo et al. (2020) systematically compared GAP, MTP, SNAP, and NNP models trained on DFT data and demonstrated that these approaches can reproduce energies, forces, elastic properties, and phonon dispersions with substantially lower computational cost than direct first-principles calculations. Their analysis also highlighted important trade-offs among accuracy, computational cost, training-data requirements, and transferability." [60].

Workflow & best practices. Developing a reliable machine-learning interatomic potential requires a diverse quantum-mechanical training dataset covering relevant structural configurations and an iterative sampling strategy to improve the model. Xue et al. (2024) created a deep-learning capability for Sc using the DP-GEN framework, combining structural relaxation, perturbation and ab-initio molecular dynamics to generate training configurations. The resulting potential was validated against DFT for structural, defect, surface and mechanical properties, demonstrating that deep-learning potentials can reproduce a range of material properties with near-DFT accuracy at substantially lower computational cost. [61].

Limitations & opportunities. When unusual but significant chemistries (such as charged defects and excited states) are absent from training data, machine learning potentials suffer; there is ongoing research into adding descriptors for long-range interactions and coupling to explicit charge models. However, with the right training, ML-IAPs can make previously unattainable reactive MD of ZnO nanostructures, defect diffusion, and large-scale morphological evolution possible. Benchmarking against DFT and experimental observables remains essential[60].

7.5 Integration of simulations with experimental synthesis

Why integration matters. There could be advantages to coupling materials design approaches with molecular-scale calculations alongside larger-scale synthesis models. Báez et al. (2021) used DFT calculations for molecular species in the ZnO hydrothermal reaction mechanism alongside a reaction-diffusion model in order to study the formation of nanoparticles. Using changes in physicochemical parameters like pH, temperature, initial concentration, and reaction rate, they managed to simulate experimentally observed ZnO shapes such as rods, sheets, and hollow spheres. [62].

Successful examples. "Wang et al. (2022) demonstrated an integrated experimental and multiscale modeling approach for ZnO nanowire-enhanced composites. ZnO nanowires were synthesized on carbon fibers using ALD and hydrothermal growth, while FESEM, EDX, XRD, and other characterization methods were used to evaluate their morphology and composition. These experimental observations were correlated with micro-homogenization, cohesive-zone modeling and finite element analysis at macro-scale to study influence of zinc

oxide nanowires on interfacial mechanical properties." [63].

Practical roadmap & future directions. The best method is to (a) create QM-level kinetic/thermodynamic data for basic processes, (b) include those rates into mesoscale growth models (phase-field, reaction-diffusion, and kMC), (c) conduct experiments based on model predictions, and (d) update/close the loop using in-situ characterisation. Reproducible, predictive ZnO materials engineering will be largely dependent on emerging methods that make integrated simulation-experiment loops more viable, such as automated workflows, high-throughput synthesis, and ML-accelerated surrogate models[60].

List of Abbreviations

DFT: Density Functional Theory	**TCNQ:** Tetracyanoquinodimethane
ML-IAP: Machine Learning Interatomic Potential	**MD:** Molecular Dynamics
TD-PBE0: Time -Dependent Perdew-Burke-Ernzerhof	**FESEM:** Field Emission Scanning Electron Microscopy
EDX: Energy Dispersive X Ray	**XRD** X-Ray Diffraction
HSE06: Heyd -Scuseria-Ernzerhof 2006	**ALD:** Atomic LAYER Deposition
DFT-U: Density Functional Theory plus Hubbard U y	**GW:** Green's Function and Screened Coulomb interaction
GAP: Gaussian Approximation Potential	**MTP:** Moment Tensor Potential
SNAP: Spectral Neighbor Analysis Potential	**NNP:** Neural Network Potential
VMC: Variational Monte Carlo	**DMC:** Diffusion Monte Carlo
ReaxFF: Reaction Force Field	**COMB:** Charge Optimized Many-Body Potential
JAX-ReaxFF: JAX -accelerated Reaction Force Field	**QM:** Quantum Mechanics
EELS: Electron Energy -Loss Spectroscop	**AIMD:** Ab Initio Molecular Dynamics
XC Functional: Exchange -Correlation Functional	**LDA:** Local Density Approximation
GGA: Generalized Gradient Approximation	

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