



Interfacial heat transport in two-dimensional heterostructures: From formation to functionality

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Abstract

Two-dimensional (2D) heterostructures provide an unusually versatile platform for engineering interfaces at the atomic scale. As these materials move toward electronic, optoelectronic and multifunctional devices, heat flow across their interfaces is emerging as a central factor that governs performance, stability and reliability. Interfacial thermal transport has traditionally been treated as a material-pair-specific conductance that should be measured and optimized. In 2D heterostructures, however, the interface is not a passive boundary with a fixed thermal response. Its conductance is shaped by the structural history, local configuration and dynamic state of the interface. In this perspective, we discuss how interface formation, thermal metrology and microscopic phonon mechanisms together define heat flow across atomically thin heterointerfaces. We highlight how direct growth and transfer assembly create distinct opportunities for lateral and vertical interfaces, how Raman thermometry, pump-probe thermoreflectance and electrical methods quantify interfacial transport, and how elastic transmission, inelastic scattering and interface-specific vibrational states govern nanoscale heat flow. We then consider how intrinsic and external control of 2D heterointerfaces can be used to tune conductance for heat dissipation, local heat confinement, rectification and thermal switching. We argue that the future of the field lies in moving from passive characterization of interfacial thermal conductance toward predictive, spatially resolved and actively controlled heat flow in 2D heterostructures.

Keywords: Two-dimensional heterostructures, interfacial thermal transport, phonon transport, thermal modulation, thermal functionality

1. Introduction

Two-dimensional (2D) heterostructures have reshaped the way interfaces are designed in condensed-matter systems. By stacking or stitching atomically thin crystals with distinct electronic structures and lattice symmetries, they create artificial materials in which charge, excitons, photons and lattice vibrations can be reorganized at the atomic scale^[1-3]. This interfacial freedom has enabled phenomena ranging from interlayer charge transfer and moiré reconstruction to tunnelling, correlated electronic phases and polar switching^[4-8]. As these systems move from model platforms toward electronic, optoelectronic and multifunctional architectures, the same interfaces that generate new physical behavior also become decisive pathways for heat flow^[9,10].

Thermal transport across 2D heterointerfaces has traditionally been described by interfacial thermal conductance (ITC), a parameter that quantifies how efficiently heat crosses a boundary between two materials^[11,12]. This description has been essential for analyzing atomically thin stacks, where heat generated by electrical bias, photoexcitation, carrier relaxation or local switching often encounters a sequence of van der Waals (vdW) gaps, lateral junctions, encapsulation layers and supporting substrates before it can be dissipated. In this conventional view, the interface is treated primarily as a thermal bottleneck whose conductance should be measured, modelled and increased.

However, 2D heterointerfaces offer a broader opportunity than this bottleneck picture suggests. Their thermal response is not determined solely by material identity, but by the local structure and state of the interface created during growth, assembly and subsequent integration^[13-16]. Unlike many conventional solid interfaces, these boundaries can often be deliberately formed, reconfigured or externally perturbed with atomic-scale sensitivity^[13,14,17]. ITC is better understood as an engineerable variable rather than a fixed descriptor of a material pair.

This change in viewpoint alters the design problem. The most useful interface is not necessarily the one with the highest thermal



conductance. High conductance may be required for rapid heat extraction, whereas reduced conductance may be useful for local heat confinement, switching or activation^[18–20]. Direction-dependent transport can enable rectification, and reversible modulation can support thermal switching or adaptive heat-flow control^[21–25]. The interface thus becomes a functional thermal element whose response can be matched to the operating requirements of the device.

This perspective is organized around this shift in viewpoint. Previous reviews have established important foundations for understanding 2D heterostructures, low-dimensional thermal transport and thermal boundary conductance across solid-solid interfaces. Here, we use 2D heterointerfaces as a model platform to ask how interfacial heat flow can be intentionally designed and eventually coupled to device function. This framing places ITC within a broader design problem, in which the interface is treated as an active object of thermal engineering.

In this perspective, we examine interfacial thermal transport in 2D heterostructures through this design-oriented lens (Figure 1). We first discuss how direct growth and transfer assembly define the formation history of an interface and set the initial conditions for heat flow. We then consider the metrology required to quantify interfacial thermal transport, followed by the microscopic mechanisms that govern elastic transmission, inelastic scattering and interface-specific vibrational states. Finally, we discuss how intrinsic and external control of 2D heterointerfaces can be used to engineer heat flow and connect thermal dissipation to thermal functionality. We argue that the next stage of the field will be defined by a transition from measuring ITC as a passive material parameter to controlling it as an actively addressable degree of freedom.

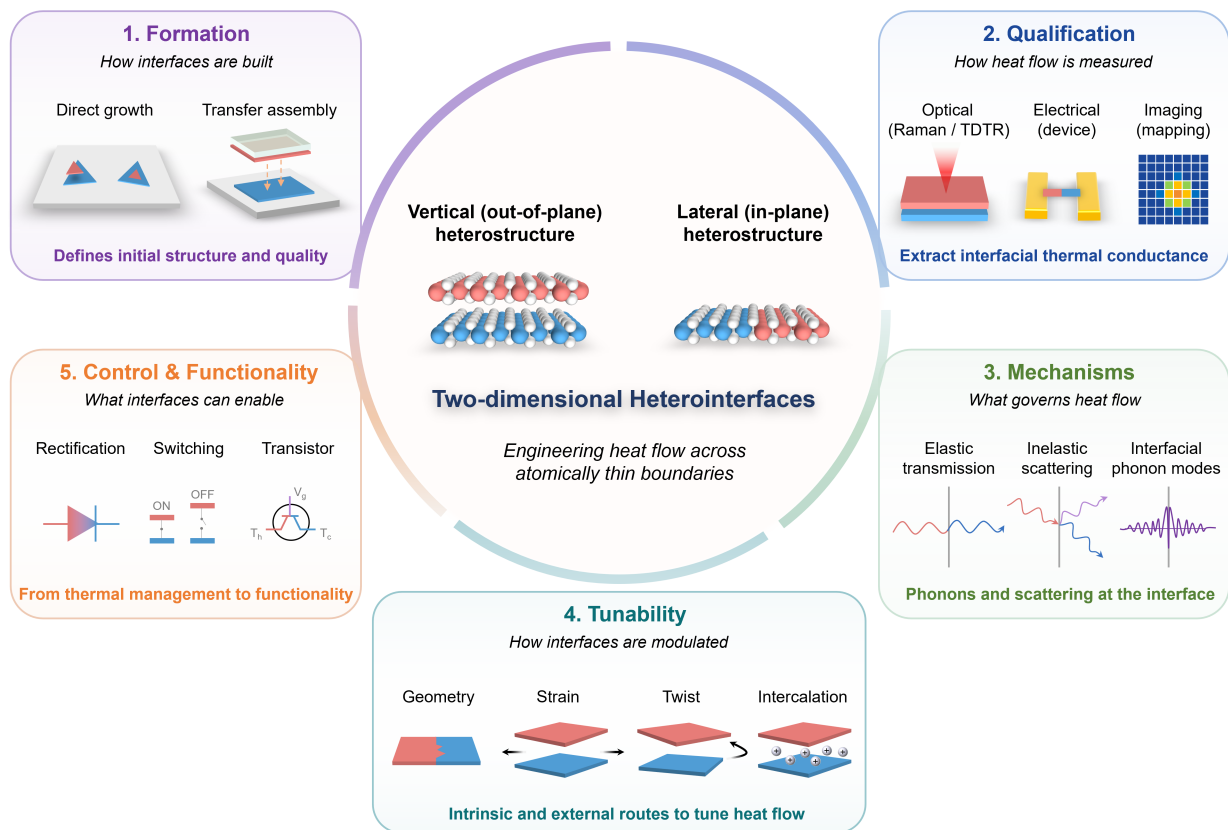


Figure 1. Interfacial heat transport in 2D heterostructures as a designable degree of freedom. 2D heterointerfaces can be formed as vertically stacked van der Waals interfaces or laterally stitched in-plane junctions. Their thermal behavior is determined by a sequence of linked processes. Interface formation through direct growth or transfer assembly defines the initial structure and quality of the boundary. Thermal metrology, including optical, electrical and mapping-based approaches, enables interfacial heat transport to be quantified. Microscopic mechanisms such as elastic transmission, inelastic scattering and interface-specific phonon modes govern how vibrational energy crosses or is redistributed at the interface. These mechanisms can be modified through intrinsic and external tuning strategies, including interface geometry, strain, twist and intercalation. When such tunability is connected to device operation, 2D heterointerfaces can move beyond passive heat dissipation toward thermal functionality, including rectification, switching and transistor-like heat-flow control. 2D: two-dimensional; TDTR: time-domain thermoreflectance.

2. Interface Formation in 2D Heterostructures

2.1 Direct growth of 2D heterostructures

The direct synthesis of 2D heterostructures has evolved from serendipitous stacking into a sophisticated paradigm of material

engineering, primarily driven by chemical vapor deposition and its advanced derivatives. The fundamental distinction between forming lateral (in-plane) versus vertical (out-of-plane) heterostructures is governed by the competition between growth kinetics and thermodynamics (Figure 2a), which together determine whether the second material forms a laterally stitched junction or a vertically stacked interface^[27,36,37]. When active species diffuse to the edge of a pre-existing crystal, lateral epitaxy is favored, whereas nucleation on the basal plane promotes vertical stacking through vdW coupling^[32,38–41]. Precursor ratio, supersaturation, and diffusion barriers can steer the nucleation pathway during growth, so lateral and vertical heterostructures are best understood as outcomes of a tunable kinetic–thermodynamic landscape rather than fixed consequences of material choice alone^[26,42].

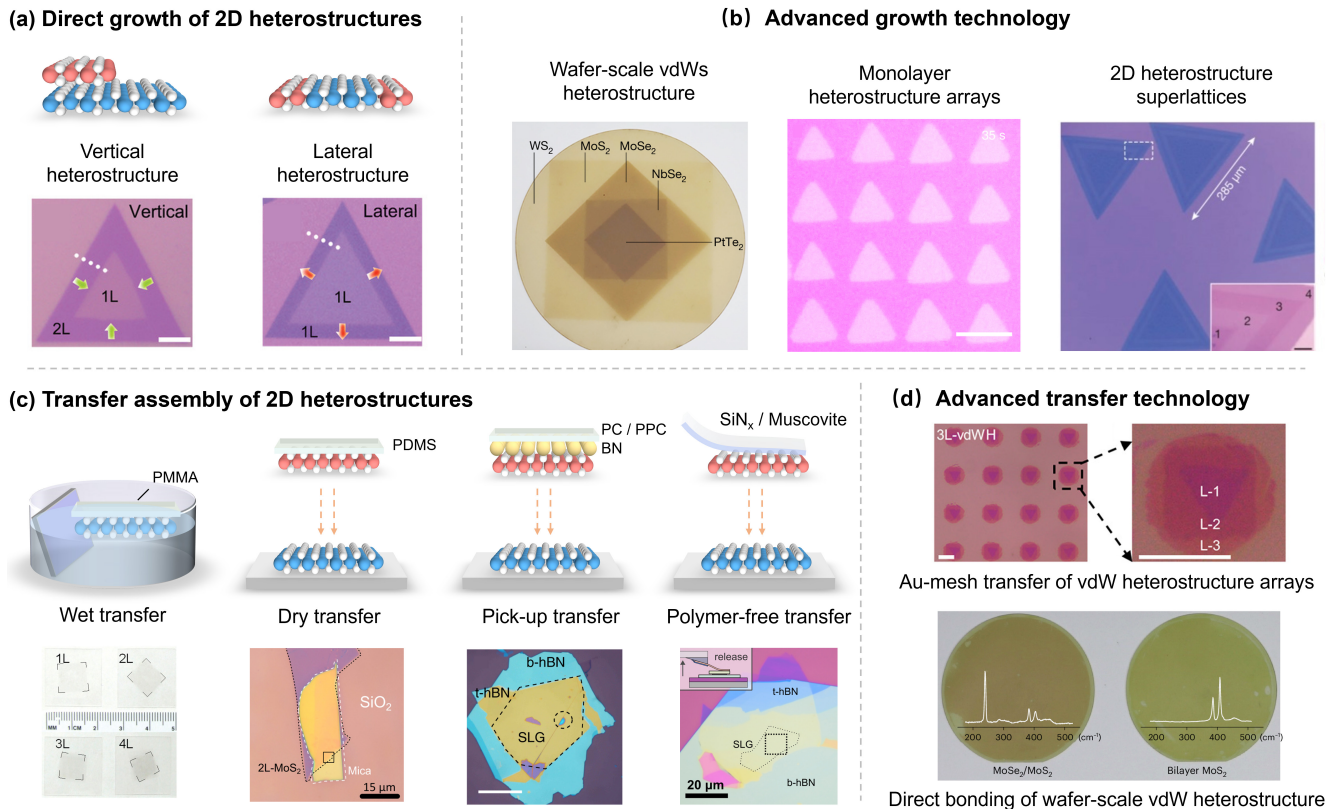


Figure 2. Formation routes and scalable assembly of 2D heterostructures. (a) Direct growth of 2D heterostructures. Representative optical images illustrate vertical and lateral growth outcomes. Reproduced with permission from reference^[26]. Copyright © 2019 John Wiley and Sons; (b) Advanced growth technologies for deterministic and large-area 2D heterostructures. Direct synthesis has progressed from isolated heterostructure flakes toward wafer-scale vdW heterostructures, monolayer heterostructure arrays and patterned 2D heterostructure superlattices, providing a route toward scalable and spatially programmable integration. Reproduced with permission from reference^[27]. Copyright © 2018 Springer Nature; reference^[28]. Copyright © 2023 Springer Nature; reference^[29]. Copyright © 2022 Springer Nature; (c) Transfer assembly of 2D heterostructures with wet transfer, dry transfer, pick-up transfer and polymer-free transfer approaches. Representative images show transferred monolayers and van der Waals stacks assembled through different transfer strategies. Reproduced with permission from reference^[30]. Copyright © 2009 American Chemical Society; reference^[31]. Copyright © 2014 IOP Publishing. Reproduced from reference^[32,33]. CC BY 4.0; (d) Advanced transfer technologies for high-throughput and wafer-scale integration. Au-mesh-assisted transfer enables patterned vdW heterostructure arrays, whereas direct bonding and debonding strategies support wafer-scale assembly of 2D semiconductor heterostructures. Reproduced with permission from reference^[34]. Copyright © 2021 American Chemical Society; reference^[35]. Copyright © 2025 Springer Nature. 2D: two-dimensional; vdW: van der Waals; PC: polycarbonate; PPC: polypropylene carbonate; BN: boron nitride; SLG: single-layer graphene.

With this degree of synthetic control, direct growth is beginning to move well beyond the production of isolated heterostructure flakes and toward a broader regime defined by both scalable fabrication and structural programmability (Figure 2b). Wafer-scale heterostructure growth is now emerging as a realistic objective, pursued through routes such as metal-film precursor transformation^[43–45], which offers a practical pathway to large-area conversion into layered heterostructures, and direct epitaxial growth^[28,46], which seeks to extend crystallographic alignment and interfacial order across macroscopic dimensions. At the same time, direct synthesis is becoming increasingly capable of producing heterostructures with prescribed spatial organization. Substrate engineering, seeded nucleation, and defect- or laser-defined growth sites are making it possible to suppress random nucleation, align domains, and position junctions with growing determinism, thereby enabling ordered heterostructure arrays rather than isolated stochastic products^[29,47]. In lateral systems, this trend reaches an even higher level of structural control in the form of superlattice growth, where periodic compositional modulation creates interface architectures that are both physically richer and synthetically more demanding than single junctions^[27,41,48,49].

The importance of these developments extends well beyond fabrication itself. Large-area growth, ordered arrays, and superlattices collectively connect interface formation to reproducibility, statistical uniformity, and device-compatible placement, all of which become essential once 2D heterostructures are viewed not as individual model systems but as scalable materials platforms. They also open a distinct scientific opportunity. In particular, laterally modulated superlattices provide an exceptional platform for exploring coherent phonon transport and other wave-like heat-transfer phenomena that are difficult to access in isolated heterointerfaces, where structural periodicity and long-range order are limited. At the same time, these advances underscore how demanding direct synthesis remains. Deterministic placement, abrupt compositional transition, high crystallinity, defect suppression, and large-area uniformity must all be achieved simultaneously within a narrow synthesis window, making direct growth not only a route to scalable heterostructures but also one of the clearest demonstrations of how demanding true interface engineering has become.

2.2 Transfer assembly of 2D heterostructures

Transfer assembly provides the complementary route to interface formation and remains the most versatile strategy for integrating 2D heterostructures, because the constituent layers can be prepared separately and then combined with substantial freedom in material choice, stacking order, lateral placement, and relative orientation. In contrast to direct growth, where the interface is defined during crystallization under a shared growth window, transfer assembly creates the interface by bringing together pre-existing surfaces through deterministic stacking, and shifts the emphasis from growth compatibility to contact formation and alignment control.

Existing transfer routes are commonly grouped into wet transfer, dry transfer, pickup-assisted transfer and polymer-free transfer (Figure 2c). Wet-transfer methods, most commonly based on sacrificial polymer supports such as PMMA, established the basic workflow for relocating exfoliated or grown 2D crystals onto target substrates and for constructing early vdW stacks^[30,50]. Their broad applicability made them foundational to the field, but also introduced persistent liabilities, including polymer residues, trapped adsorbates, wrinkles, and interfacial contamination^[51]. Dry-transfer methods, typically implemented with viscoelastic stamps such as polydimethylsiloxane^[31], polypropylene carbonate^[52], or polycarbonate^[32], reduced liquid exposure and markedly improved placement control, thereby becoming the basis of deterministic vdW assembly. Pickup-based approaches, especially h-BN-assisted pickup and hot-pickup strategies, advanced interface quality further by ensuring that buried internal interfaces are never directly exposed to sacrificial polymers or solvents^[53,54]. More recently, low-contamination and polymer-free variants, including flexible SiN_x-membrane and muscovite crystal platforms, have further expanded this toolbox by improving interface cleanliness while preserving the positional and rotational precision required for designed heterostructures^[33,55]. These increasingly directional and contamination-minimized transfer routes have become particularly important for high-quality vdW heterostructures because they enable cleaner encapsulation, greater reproducibility, and precise twist-angle control, all of which are indispensable for twistronics and designer heterostacks.

Recent developments also make clear that transfer assembly is no longer confined to laboratory-scale manipulation of isolated flakes, but is beginning to evolve into a technologically meaningful route for large-area integration (Figure 2d). Dry exfoliation of large-area monolayers and heterostructure arrays has shown that transfer can be coupled to scalable preparation strategies capable of producing ordered 2D building blocks well beyond individual crystals^[34,56,57]. At the same time, direct bonding and debonding of 2D semiconductors points to a more advanced paradigm in which epitaxially grown 2D semiconductor wafers can be bonded, released, and re-integrated without reliance on conventional adhesive-mediated transfer, thereby bringing 2D heterostructures closer to wafer-level processing and heterogeneous device integration^[35]. These advances suggest that the future of transfer assembly will be defined not only by cleaner interfaces, but also by closer compatibility with semiconductor manufacturing. This shift is especially consequential because when transfer technologies become cleaner, more uniform, and more wafer-compatible, they cease to be merely convenient stacking tools and instead begin to function as enabling platforms for deliberately engineering ITC in integrated devices.

2.3 Interface formation as the starting point of thermal design

The thermal consequences of these formation routes arise from the interfacial structures they leave behind. In transfer-assembled vdW stacks, polymer residues, trapped adsorbates, wrinkles and local delamination can increase the effective interlayer spacing, reduce the real contact area and introduce spatially nonuniform coupling, thereby broadening or lowering the extracted ITC^[58-62]. Cleaner pickup and polymer-free transfer can mitigate these effects by producing more intimate and reproducible layer-to-layer contact. In directly grown lateral heterostructures, the relevant structural variables are different. Edge disorder, dislocations, reconstructed motifs and alloyed transition regions define the width, bonding topology and chemical abruptness of the in-plane boundary, which can determine whether the interface behaves as a sharp phonon reflector, a diffuse transition layer or a selective vibrational filter^[63-66].

These contrasting formation routes give rise to distinct scientific opportunities. Direct growth lays the foundation for scalable device integration and, by enabling sharp covalent interfaces, provides access to nanoscale phonon phenomena such as confinement, coherence, and tunnelling at chemically stitched boundaries. Transfer assembly, by contrast, opens an unprecedented opportunity to

study phonon transport across vdW heterointerfaces because the interface itself can be deliberately reconfigured to produce new transport regimes and functionalities. From the perspective advanced in this article, neither route is intrinsically superior. Direct growth is likely to remain central to scalable integration and intrinsically sharp interface physics, whereas transfer assembly will remain the more powerful route for discovering and engineering tunable phonon transport in vdW systems. The future of the field will depend on using these two formation routes in complementary ways to transform 2D heterointerfaces from passive thermal boundaries into actively designable thermal elements.

3. Quantifying Interfacial Thermal Transport in 2D Heterostructures

Quantifying interfacial thermal transport in 2D heterostructures is challenging because the heat-carrying interface is atomically thin, weakly accessible and embedded within a complex multilayer environment. The thermal signal from a single heterointerface is often small, while the measured response inevitably contains contributions from the adjoining 2D layers, metal contacts, encapsulation layers and supporting substrates. In vertical stacks, the interface of interest is frequently buried beneath the surface, while in lateral heterostructures, heat must be driven and detected across a nanoscale in-plane boundary. As a result, reliable quantification requires both sensitive thermometry and careful control of optical absorption, heat-flow geometry, background thermal resistances and model parameter coupling.

3.1 Raman thermometry

Raman thermometry has been one of the most widely used approaches for 2D materials since the landmark optothermal Raman measurements on monolayer graphene established the method as a noncontact route to thermal characterization^[67-69]. Its basic principle is to infer temperature from Raman peak shifts while laser heating drives the thermal response (Figure 3a). A particular advantage in 2D heterostructures is the fingerprint nature of Raman spectroscopy, which often allows the temperature rise of different constituent layers to be measured separately within the same vdW stack^[70]. This layer selectivity makes it possible to directly determine the temperature difference between adjacent layers and thereby access interfacial thermal transport with a level of physical specificity that is difficult to achieve in many other optical methods^[58,71-74]. This capability has also been extended to electrically driven heterostructures, where integrated Joule heating combined with layer-resolved Raman thermometry enables the thermal resistance between individual 2D monolayers in a vdW stack to be identified directly^[70,75,76].

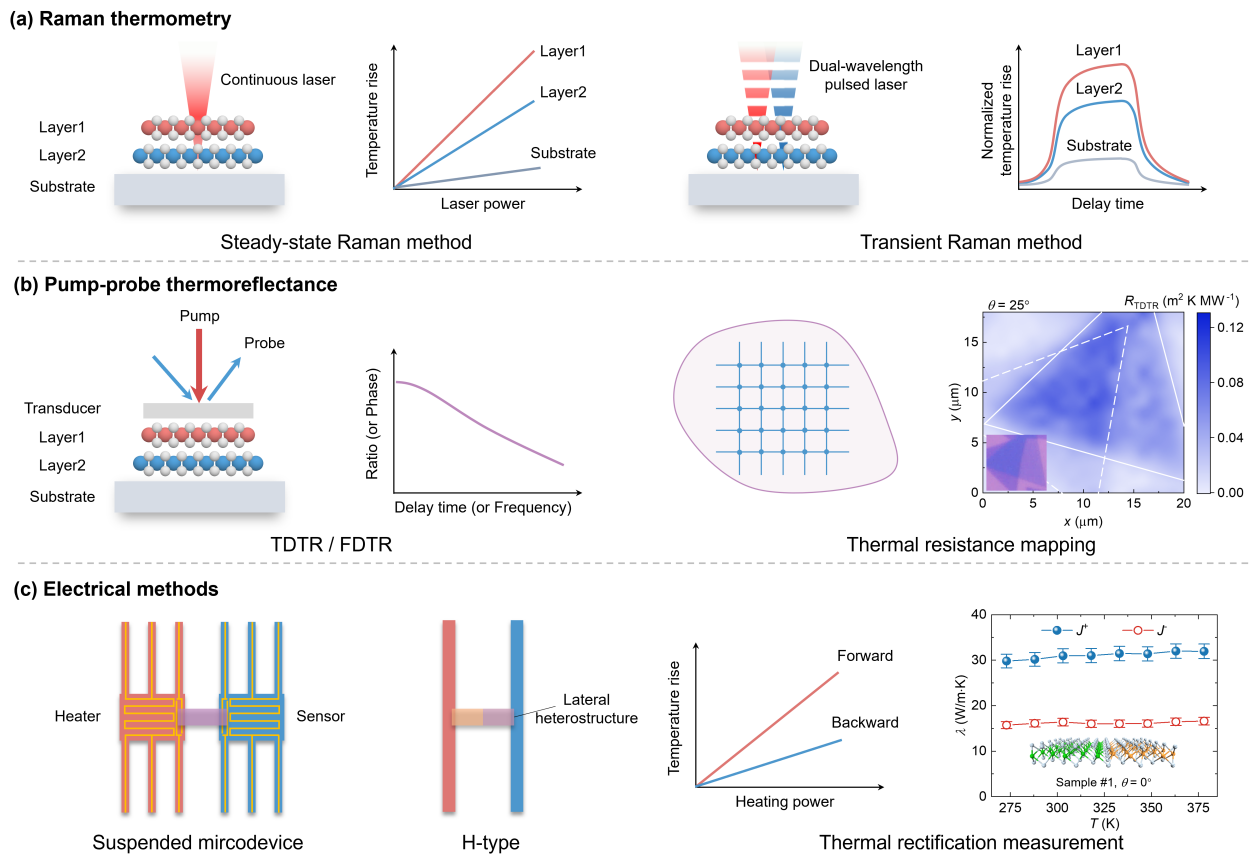


Figure 3. Experimental approaches for quantifying interfacial thermal transport in 2D heterostructures. (a) Raman thermometry methods. In steady-state Raman thermometry, a continuous laser simultaneously heats and probes the heterostructure, and the temperature rise of different layers or the substrate is extracted from Raman peak shifts as a function of laser power. In transient Raman thermometry, pulsed or dual-wavelength excitation tracks the time-dependent thermal response, reducing

reliance on laser absorption coefficient; (b) Pump-probe thermoreflectance methods. In TDTR and FDTR measurements, a pump beam periodically heats a metal transducer deposited on the heterostructure, while a delayed probe beam monitors the transient reflectance response. Fitting the delay- or frequency-dependent signal with a multilayer heat-transfer model enables extraction of interfacial thermal resistance. Spatial scanning further allows thermal resistance mapping across large-area 2D heterostructures. Reproduced with permission from reference^[13]. Copyright © 2026 National Academy of Sciences; (c) Electrical thermal metrology. Suspended microdevice platforms measure heat flow through a sample bridging calibrated heater and sensor membranes, enabling high-accuracy thermal conductance measurements. H-type devices provide a simpler geometry for probing directional heat flow across lateral heterostructures and can be used to quantify forward and backward thermal transport, including thermal rectification. Reproduced with permission from reference^[24]. Copyright © 2022 National Academy of Sciences. 2D: two-dimensional; TDTR: time-domain thermoreflectance; FDTR: frequency-domain thermoreflectance.

The main limitation is that the absorbed laser power is often difficult to determine accurately, especially in supported multilayer stacks, which directly limits quantitative accuracy^[77–79]. This challenge has motivated the development of transient optothermal Raman, including state-differential Raman^[80,81], flash Raman^[82,83] and dual-wavelength flash Raman^[84,85] schemes, which reduce dependence on absolute absorption and improve sensitivity to interfacial transport (Figure 3a). Even so, Raman methods remain intrinsically better suited to situations in which heat diffuses away from the laser-heated region in a relatively symmetric manner, and are much less straightforward for quantifying heat conduction across lateral heterointerfaces. Under such conditions, dual-wavelength Raman approaches that enable spatial mapping of the in-plane temperature field during laser heating may provide a viable pathway toward overcoming this limitation^[86].

3.2 Pump-probe thermoreflectance

Time-domain thermoreflectance (TDTR) and frequency-domain thermoreflectance (FDTR) have become standard tools for quantifying heat transfer in thin films and interfaces^[87,88]. Their basic principle is to use modulated optical heating and reflectance-based thermometry to probe transient or frequency-dependent thermal response (Figure 3b), which is then interpreted through a multilayer heat-transfer model^[89–91]. For 2D heterostructures, these methods are particularly well suited to supported vertical stacks, where the thermally relevant interface is buried beneath the surface and the dominant process of interest is cross-plane heat flow rather than lateral diffusion.

A major strength of pump-probe thermoreflectance is its combination of interface sensitivity and experimental throughput^[92–97]. Because the technique directly tracks the thermal response of the multilayer stack without requiring full spectral acquisition at every position, it is well suited to rapid spatial mapping over extended sample areas, which is especially valuable for 2D heterostructures whose interface quality and thermal coupling are often spatially nonuniform^[95,98]. This capability has recently enabled mapping-based studies of twisted vdW heterointerfaces (Figure 3b), including the observation of anomalously enhanced ITC in MoS₂/WS₂ heterobilayers^[13]. These strengths are balanced by well-known limitations. Interpretation is strongly model dependent, parameter covariance in multilayer fitting can be substantial, and conventional implementations usually require a metal transducer layer that may perturb the native interface^[90]. In addition, the measured signal represents a finite subsurface sampling volume rather than an atomically localized interface, which can become a significant issue in strongly heterogeneous systems^[99]. For this reason, recent transducerless, wideband, and beam-offset variants are especially relevant to 2D materials^[100–103], where buried-interface sensitivity, spatial mapping, and reduced measurement perturbation are all important.

3.3 Electrical methods

Electrical thermal metrology remains one of the most accurate routes for quantifying heat transport in suspended low-dimensional systems. In its classical form, the suspended microdevice or suspended micro-bridge approach measures heat flow between two thermally isolated membranes bridged by the sample (Figure 3c), thereby defining a relatively well-controlled thermal circuit and enabling high-precision extraction of thermal conductance or thermal conductivity^[104,105]. This framework has been central to the measurement of low-dimensional materials because it minimizes parasitic substrate leakage and directly links the applied heating power to the resulting temperature response through calibrated electrical sensing^[106–109].

For 2D heterostructures, the importance of electrical methods extends beyond accuracy. Unlike optical approaches, which are naturally best matched to laser-driven diffusion around a local heating spot, electrical methods are inherently compatible with directional heat-flow geometries. This makes them particularly valuable for lateral heterostructures, where the central question is often how efficiently heat is transmitted across an in-plane interface. In this sense, electrical metrology helps fill a critical gap left by optical methods by providing a more direct route to quantifying cross-interface heat conduction in laterally stitched junctions. This capability has become especially important in studies of thermal rectification and electrically driven reversible phonon transport, where heat must be driven and sensed along two opposite directions through the same heterointerface^[110–112].

Within this family, H-type device configurations are especially useful in this regard because they establish a device-oriented fabrication paradigm in which sensor structures can be integrated directly with the heterostructure, making the method practical for small or fragile interfaces that are difficult to study in conventional suspended-membrane architectures (Figure 3c)^[17,24,113–116]. This is particularly valuable for lateral heterojunctions and other integrated 2D devices, where the thermally relevant interface may be too

small or too difficult to manipulate reliably within a conventional suspended-membrane architecture^[24,113]. The principal limitations of electrical methods remain fabrication complexity, thermal contact resistance between the sample and electrodes, and parasitic heat loss through radiation, metal leads, or residual substrate coupling. However, for many 2D heterostructures, these limitations are offset by the fact that electrical platforms provide one of the most direct ways to probe directional phonon transport across a specific interface under device-relevant conditions.

Table 1 summarizes the main experimental approaches for quantifying interfacial thermal transport in 2D heterostructures. These methods differ in their suitable interface geometry, extracted thermal quantity, probing scale, and dominant sources of uncertainty. The comparison highlights that ITC is usually inferred from a broader thermal response rather than measured as an isolated interface property, making method selection and uncertainty analysis central to reliable quantification.

Table 1. Comparison of experimental methods for quantifying interfacial thermal transport in 2D heterostructures.

Method	Suitable geometry	Main extracted quantity	Probing scale	Main uncertainties
Steady-state Raman method	Suspended/supported vertical heterostructures	Thermal conductivity, ITC	Optical spot size, usually sub- μm to μm	Laser absorption, Raman temperature calibration and laser spot profile
Transient Raman method		Thermal diffusivity, ITC		Weak transient Raman signal and laser spot profile
TDTR/FDTR	Supported vertical heterostructures	In-plane/cross-plane thermal conductivity, ITC	Pump/probe spot and thermal penetration depth, typically μm lateral scale and tens of nm to μm depth scale	Model dependence parameter covariance, transducer thickness and thermal properties
Suspended microdevice method	Suspended lateral heterostructures	Directional thermal conductance, Thermal rectification ratio	Device-defined in-plane path, typically μm scale	Fabrication complexity, thermal contact resistance and radiative heat loss
H-type method				Fabrication complexity, thermal contact resistance and parasitic heat leakage through metal leads

2D: two-dimensional; ITC: interfacial thermal conductance; TDTR: time-domain thermoreflectance; FDTR: frequency-domain thermoreflectance.

3.4 Outlook for future metrology

The most consequential advances in this area are likely to come from metrologies that are simultaneously spatially resolved, high-resolution, time-resolved, and operando. In practice, spatial mapping and spatial resolution are closely linked. Many of the most interesting structural motifs in 2D heterostructures, including moiré superlattices^[117], reconstructed boundaries^[118], one-dimensional (1D) channels^[119], and nanoscale hot spots in operating devices^[120], fall below the spatial scale of conventional optical thermal probes. This motivates the convergence of thermal metrology with near-field and scanning-probe methods, such as tip-enhanced Raman methods^[117,121] and optical pump-probe-inspired atomic force microscopy schemes^[122]. A related opportunity lies in coupling electrical and optical methods. Electrical techniques remain well suited to driving directional heat flow across lateral heterointerfaces, whereas optical readout is better suited to imaging the resulting temperature field^[123]. Higher spatial resolution will also be increasingly important for measuring local junction temperatures in 2D devices, where nanoscale thermal nonuniformity may strongly influence switching, reliability, and functional stability.

Time resolution is likely to become equally important. If tunable interfacial conductance is to support thermal switches, thermal transistors, or dynamically reconfigurable heat management, then metrology must move beyond static or quasi-static characterization toward opto-electrical hybrid measurements, in which electrical driving and optical or local thermal readout are combined to resolve how interfacial heat flow evolves in real time. The objective is to capture how that parameter changes under gate bias, current flow, optical excitation, structural relaxation, or other external fields^[25,124]. In this broader sense, the future of thermal metrology will depend on bridging large-area mapping, nanoscale spatial resolution, and real-time operando measurement within a single experimental framework.

4. Mechanisms of Heat Flow Across Atomically Thin Heterointerfaces

Interfacial heat transport at the nanoscale differs fundamentally from that across conventional bulk interfaces^[11,125,126]. At atomically thin heterointerfaces, heat flow depends not only on the bulk properties of the adjoining materials, but also on the microscopic structure of the interface itself, including bonding topology, local registry, and spatial heterogeneity. This is especially true for 2D heterostructures, where weak vdW coupling, moiré reconstruction, interfacial corrugation, and low-dimensional confinement all amplify the role of local interfacial physics. Atomically thin heterointerfaces also often lie outside the assumptions of simple diffuse or continuum heat flow. At nanoscale interfaces, the boundary can selectively transmit, reflect, convert, or localize vibrational energy. Interfacial heat transport becomes highly sensitive to vibrational spectral overlap, bond stiffness contrast, interfacial force constants, and interface-specific phonon modes (Figure 4a).

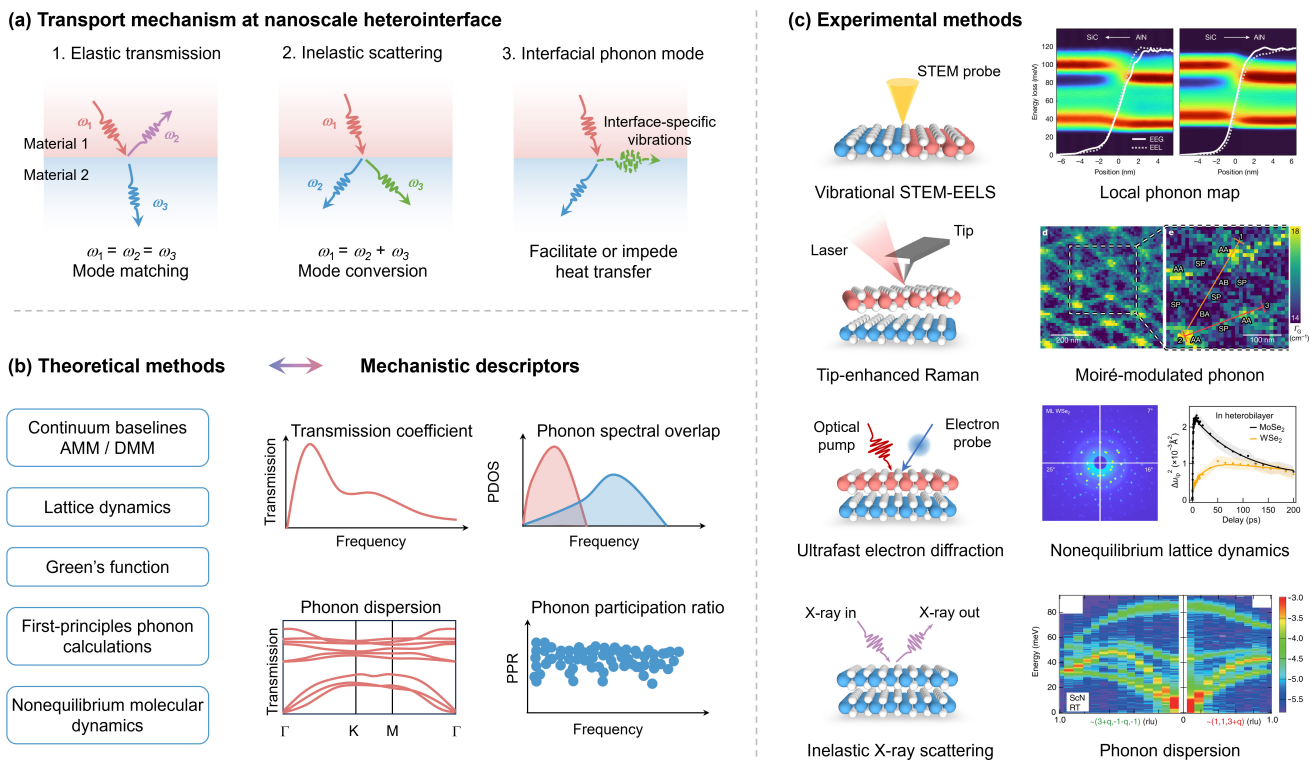


Figure 4. Mechanistic understanding of heat flow across nanoscale heterointerfaces. (a) Transport mechanisms at nanoscale heterointerfaces. Elastic transmission occurs when an incident phonon transmits across the interface without changing frequency, provided that vibrational modes on the two sides are sufficiently matched. Inelastic scattering allows energy transfer through mode conversion, in which an incident phonon couples to multiple modes with different frequencies. Interface-specific phonon modes can further localize vibrational energy at the boundary and either facilitate or impede interfacial heat transfer; (b) Theoretical methods for analyzing interfacial heat transport mechanisms. Continuum models, lattice dynamics, Green's-function approaches, first-principles phonon calculations and nonequilibrium molecular dynamics provide complementary descriptions of interfacial phonon transport. Their outputs include transmission coefficients, phonon spectral overlap, phonon dispersion and phonon participation ratios, which help identify whether heat flow is governed by harmonic matching, inelastic scattering, localized vibrational modes or structural disorder; (c) Experimental methods for probing interfacial phonon dynamics. Vibrational STEM-EELS provides nanoscale phonon mapping near interfaces, tip-enhanced Raman spectroscopy resolves moiré-modulated and localized vibrational modes, ultrafast electron diffraction tracks nonequilibrium lattice dynamics, and inelastic X-ray scattering measures phonon dispersion and collective excitations. Reproduced from reference^[127,128]. CC BY 4.0. Reproduced with permission from reference^[117]. Copyright © 2021 Springer Nature; reference^[129]. Copyright © 2018 American Physical Society. STEM: scanning transmission electron microscopy; EELS: electron energy loss spectroscopy; AMM: acoustic mismatch model; DMM: diffuse mismatch model.

4.1 Core transport mechanisms at nanoscale heterointerfaces

The most basic starting point for understanding interfacial heat transport is elastic vibrational transmission^[130,131]. In this picture, phonons transfer energy across the interface when modes on the two sides are compatible in frequency, polarization, and velocity. Elastic transmission is most effective when the adjoining materials have overlapping low-frequency phonon spectra, comparable acoustic impedances, and an ordered interface that preserves efficient coupling between incident, reflected, and transmitted modes. This framework captures the importance of vibrational matching and helps explain why interfaces with better low-frequency overlap often exhibit higher thermal conductance^[132,133]. For 2D heterostructures, it is especially relevant to long-wavelength acoustic modes and to out-of-plane vibrations that couple directly across vertically stacked layers^[9,13,94].

Elastic transmission, however, is rarely sufficient on its own. When the two materials are strongly mismatched in their vibrational spectra, local anharmonicity is large, or interface disorder relaxes momentum selection, inelastic phonon scattering becomes increasingly important^[134-138]. Rather than requiring one-to-one mode matching, inelastic processes redistribute thermal energy among different phonon branches during transmission and can open channels inaccessible within a purely harmonic picture. Such processes can substantially enhance heat transfer across mismatched interfaces, especially in atomically thin systems where broken symmetry, local reconstruction and interface-specific perturbations strengthen mode conversion^[13,15].

A further level of complexity arises from interfacial phonon modes and localized interface vibrations^[139-143]. These excitations are generated or strongly reshaped by the interface itself rather than simply inherited from either adjoining material. Their influence on heat flow depends on whether they act as bridge states or trapping states. Modes that overlap spectrally and spatially with phonons on both sides of the interface can mediate mode conversion and facilitate interfacial energy transfer, whereas highly localized modes that couple strongly to only one side tend to trap vibrational energy and enhance reflection or diffuse scattering. At the nanoscale, the interface is not merely a filter for bulk phonons, but can also host vibrational states with their own thermal role.

These general mechanisms take different forms in vertical and lateral 2D heterointerfaces. For vertical heterointerfaces, the central issue is cross-plane energy transfer across a weakly bonded interlayer gap. Because adjacent layers are linked primarily through vdW interactions, transport depends strongly on interfacial force constants, local spacing, and the extent of real contact^[61,144]. Twist and lattice mismatch further modulate local atomic registry and generate moiré reconstruction, so that heat flow is governed by a spatially varying landscape of interfacial coupling and nonequilibrium mode populations^[117].

Lateral heterointerfaces are governed by a different physical setting. Here heat does not cross a weakly bonded gap, but propagates through a chemically stitched or reconstructed transition region within the plane. The decisive factors become the width and atomic structure of that boundary, including mass contrast, bond-stiffness variation, alloying, defects, and 1D interface motifs^[66,145,146]. Depending on how the junction is formed, the interface may behave as a sharp phonon reflector, a distributed transition layer, or a selective vibrational filter^[24].

4.2 Theoretical methods for analyzing interfacial heat transport mechanisms

Mechanistic understanding has relied on a combination of theoretical and atomistic tools. At the most approximate level, acoustic and diffuse mismatch models remain useful as baseline descriptions of interfacial transmission^[130,131]. Their value lies mainly in the physical intuition they provide, but for atomically thin heterointerfaces, where local registry, weak bonding, reconstruction, and interface-specific vibrational states all become important, such continuum-level treatments are rarely sufficient on their own.

More detailed insight typically comes from lattice dynamics^[147,148], Green's function approaches^[149,150], first-principles phonon calculations^[151,152], and nonequilibrium molecular dynamics^[153-155]. These methods resolve phonon transmission spectra, spectral heat flux, local density of states, interfacial force constants, mode-resolved contributions, and the role of anharmonicity (Figure 4b). In doing so, they shift the question from the extraction of a single conductance value to a more revealing set of issues, namely which modes carry heat, where scattering occurs, and how specific structural features modify the available transport pathways.

For 2D heterostructures, descriptors such as spectral overlap factors^[132,156], phonon participation ratios^[157,158], and mode-resolved transmission coefficients^[135,159] have become especially useful for distinguishing whether an observed trend originates primarily from harmonic matching, stronger interlayer coupling, enhanced inelastic scattering, or interface-specific vibrational states (Figure 4b). These descriptors should be interpreted together because a single trend in ITC may reflect several coupled mechanisms. Spectral overlap, for example, captures the availability of vibrational states for elastic exchange, but it does not determine transmission unless interfacial coupling, polarization, group velocity, and real contact quality are also considered.

4.3 Experimental methods for analyzing interfacial heat-transport mechanisms

Experimental access to interfacial heat-transport mechanisms remains challenging because the relevant phonons are often highly localized in space, evolve on ultrafast timescales, and are embedded in structurally complex interfaces (Figure 4c). Among the emerging approaches, vibrational scanning transmission electron microscopy (STEM)-electron energy loss spectroscopy (EELS) has become especially promising^[160,161]. By combining electron microscopy with vibrational spectroscopy, it can access phonon-related excitations with nanometer and, in favorable cases, sub-nanometer spatial resolution, making it unusually well suited to reconstructed interfaces, defect-rich boundaries, and other localized motifs central to nanoscale heat transport^[142,162-164]. Recent studies have gone beyond static vibrational imaging to probe phonon transport dynamics across interfaces directly, indicating that electron microscopy can begin to resolve where temperature drops and inelastic scattering are concentrated at nanometer scales^[127].

A broader experimental landscape is also beginning to take shape. Ultrafast electron diffraction and diffuse-scattering methods provide femtosecond access to nonequilibrium lattice dynamics and have been used to follow interlayer energy flow and coherent acoustic phonon evolution in layered systems^[128,165,166]. Tip-enhanced Raman spectroscopy has shown that moiré-modulated lattice dynamics can be visualized below the diffraction limit, as demonstrated by nano-Raman imaging of localized phonon behavior in

low-angle twisted bilayer graphene^[117]. Momentum-resolved probes, including inelastic X-ray scattering and resonant inelastic X-ray scattering, provide a complementary perspective by resolving phonon dispersion and other lattice excitations in reciprocal space^[129,167-169]. Although these methods are not yet routine thermal metrologies in the conventional sense, they increasingly allow the field to probe the phonons themselves rather than infer their role only through effective thermal parameters.

4.4 Outlook for mechanistic studies of interfacial heat transport

Mechanistic studies are likely to move first from idealized interfaces toward formed interfaces, meaning models and measurements that explicitly incorporate growth history or transfer history. A parallel shift will be from average descriptors toward interface-specific excitations. The field is moving from asking only how much heat crosses an interface to asking which phonons carry that heat, how they are transformed, and where their transport is spatially concentrated. Methodologically, predictive understanding will require multiscale theoretical frameworks that preserve atomistic realism while remaining tractable on experimentally relevant length and time scales. This is where machine-learning interatomic potentials are becoming especially important^[170,171]. Conventional empirical potentials are often too rigid to capture weak interlayer coupling, registry dependence, and strongly structure-sensitive interface dynamics with sufficient fidelity, whereas first-principles methods remain too computationally expensive for realistic nonequilibrium simulations. Machine-learning interatomic potentials provide a route between these limits by retaining near-first-principles accuracy while extending simulations to much larger systems and richer structural landscapes. More broadly, the future of this area will depend on tighter integration between theory and experiment, so that interface phonons and nonequilibrium lattice dynamics can be observed directly and interpreted in structurally realistic models. The longer-term opportunity is to establish a predictive framework in which interfacial heat transport can be designed through control of bonding topology, local registry, morphology, and external perturbation.

5. Engineering Interfacial Heat Flow for Device Functionality in 2D Heterostructures

If interfacial heat transport in 2D heterostructures is governed by local bonding, interfacial morphology, and vibrational coupling, then the natural next question is how those quantities can be deliberately controlled. For vdW heterostructures, this question is especially compelling because the interface remains structurally accessible even after the constituent layers have been assembled. In this sense, interface engineering can become the attempt to identify which features of the interface are written into it during formation, which can be modified afterward, and how these control approaches can be used to shape heat flow in a reproducible and functionally meaningful way.

5.1 Engineering interfacial heat flow through intrinsic and external control

For vertical heterointerfaces, a useful starting point is to distinguish between intrinsic structural and chemical tuning and external, potentially reversible tuning. The first class includes factors such as local registry, defects, doping, and interfacial chemistry (Figure 5a). These variables define the interfacial state at a more fundamental level because they are embedded in the composition or local bonding environment of the junction itself. Local registry determines how atomic motion is coupled across the interface at the smallest scale^[61,144]. Defects and dopants can alter vibrational spectra, broaden available scattering channels, or change local force constants^[172-175]. Interfacial chemistry and functionalization may further shift selected regions of a junction away from the purely vdW limit and toward mixed bonding environments with stronger local coupling^[176,177]. Such factors are often introduced during growth, assembly, or post-processing, and are better viewed as parameters written into the interface than as variables that can be continuously tuned afterward^[178-180].

A second class of control is more distinctive to vdW heterostructures because it acts on the interface from the outside and can be made reversible (Figure 5b). Twist is the clearest example^[95,181,182]. By changing relative rotational alignment without changing composition, twist reshapes local stacking registry, transforms a nominally uniform interface into a laterally modulated coupling landscape, and reconfigures the phonon scattering channels^[13,94,96,183]. Strain provides a similarly powerful route by altering phonon dispersion, interlayer spacing, and local contact pressure^[184,185]. Ion intercalation offers another potentially powerful means of control by modifying interlayer separation, charge environment, and vibrational coupling through species inserted between adjacent layers^[186-190]. Its ability to strongly modulate interfacial thermal transport has so far been explored mainly in homogeneous or symmetric layered systems, whereas its extension to heterostructures remains largely open. The broader significance of these external routes is that they preserve the idea of the interface as a thermally active element rather than a static boundary.

The control problem is different for lateral covalent heterointerfaces. In this case, the interface is not a weakly bonded gap between stacked layers, but a chemically stitched in-plane boundary through which heat must propagate. The most consequential design variables are the abruptness of elemental transition, the width and structure of the interfacial region, and the angle between the boundary and the imposed heat-flow direction (Figure 5c)^[24,32,38,40,41,191,192]. A sharp interface, a diffuse alloyed transition, and a boundary containing extended defects or reconstructed motifs will not present the same phonon landscape to an incoming heat current^[9,66,193-195]. Their significance is further enhanced by the fact that lateral 2D heterointerfaces often possess an intrinsic structural asymmetry along the heat-flow direction. This makes them especially attractive for thermal rectification, because forward and reverse heat flow can experience different phonon scattering landscapes across the same boundary^[24,110,196-198]. This asymmetry is

often more directly expressed than in vertically stacked vdW interfaces, because heat in a lateral junction must traverse an in-plane boundary whose composition and bonding can differ along the forward and reverse directions. In this sense, lateral heterostructures provide a particularly promising platform for realizing direction-sensitive thermal functions in atomically thin systems.

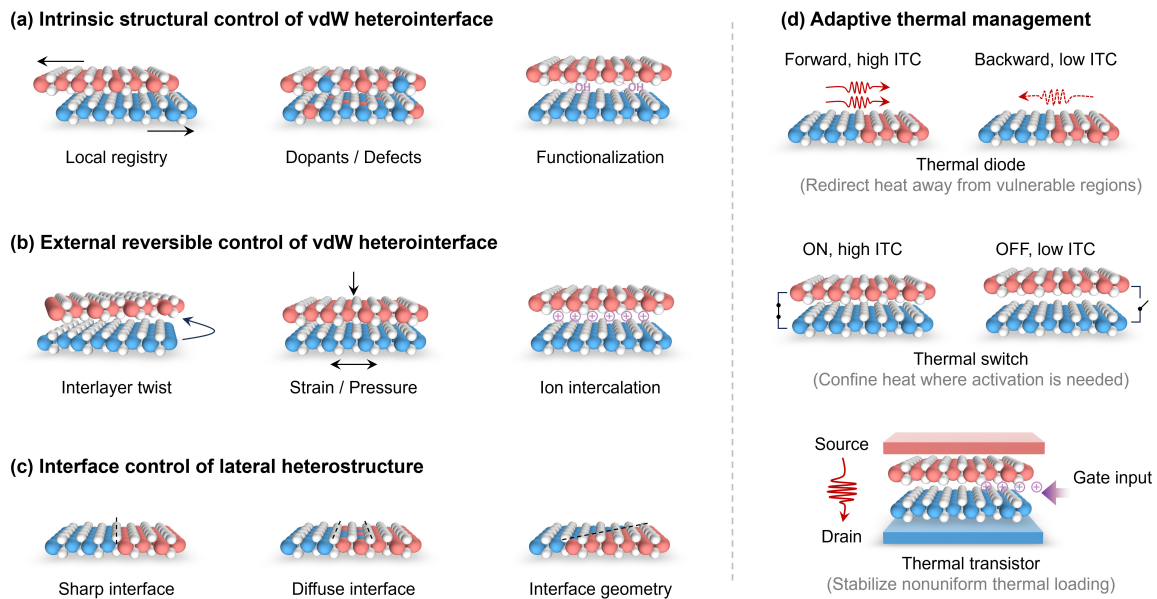


Figure 5. Engineering interfacial heat flow toward adaptive thermal functionality in 2D heterostructures. (a) Intrinsic structural control of vertical vdW heterointerfaces. Local registry, dopants or defects, and interfacial functionalization modify the local bonding environment, vibrational coupling and phonon-scattering landscape across the interface, thereby defining thermal transport properties that are largely written into the junction during growth, assembly or post-processing; (b) External and reversible control of vdW heterointerfaces. Interlayer twist, strain or pressure, and ion intercalation provide routes to reconfigure interfacial spacing, contact, charge environment and phonon coupling after the heterostructure has been formed. These perturbations can potentially enable dynamic modulation of ITC; (c) Interface control in lateral heterostructures. In-plane heterointerfaces can be engineered through the abruptness of the elemental transition, the width of a diffuse interface and the geometry of the boundary. Because heat must propagate across a chemically stitched and often asymmetric in-plane junction, lateral heterostructures provide a natural platform for direction-dependent heat flow and thermal rectification; (d) Adaptive thermal-management concepts enabled by tunable heterointerfaces. A thermal diode allows forward heat flow with high ITC while suppressing backward transport. A thermal switch reversibly toggles between high- and low-conductance states to confine or release heat as needed. A thermal transistor uses an external gate input to modulate heat current between source and drain, providing a route toward active control of nonuniform thermal loading. 2D: two-dimensional; vdW: van der Waals; ITC: interfacial thermal conductance.

Representative values further illustrate the broad range of interfacial heat-transport magnitudes and modulation responses in 2D heterointerfaces (Table 2). For vertical vdW interfaces, reported ITC values range from only a few $\text{MW m}^{-2} \text{K}^{-1}$ in weakly coupled or highly mismatched stacks to several tens of $\text{MW m}^{-2} \text{K}^{-1}$ when contact quality, encapsulation, or interfacial coupling is improved. External perturbations such as twist, strain, and intercalation can further modify the effective conductance by changing spectral overlap, interlayer spacing, and disorder. For lateral covalent interfaces, directly measured ITC values remain less common, and many studies instead report effective in-plane thermal conductance, thermal conductivity variation, or thermal rectification. Even so, these results show that boundary abruptness, defect structure, composition profile, and interface geometry can strongly influence phonon transmission across chemically stitched junctions. The values summarized in Table 2 are merely intended as representative benchmarks, and direct comparison should take into account differences in interface geometry, measurement protocol, and reported thermal quantity.

Table 2. Representative interfacial thermal transport values and modulation effects in 2D heterointerfaces.

Interface type	Representative system and control route	ITC value or modulation magnitude	Measurement or simulation method	Control mechanism	Ref.
vdW interface	Gr/MoS ₂ heterobilayer	$11 \pm 3 \text{ MW m}^{-2} \text{K}^{-1}$	Steady-state Raman	/	[70]
	Gr/WSe ₂ heterobilayer	$5 \pm 3 \text{ MW m}^{-2} \text{K}^{-1}$			
	MoS ₂ /WSe ₂ heterobilayer	$9 \pm 3 \text{ MW m}^{-2} \text{K}^{-1}$			
	Monolayer WS ₂	$7 \text{ MW m}^{-2} \text{K}^{-1}$	TDTR		[91]

Covalent interface	/multilayer h-BN				
	Monolayer WSe ₂				
	/multilayer h-BN				
	Multilayer Gr/h-BN	98.0 ± 7.6 MW m ⁻² K ⁻¹	NEMD		[144]
	Monolayer MoS ₂	74 ± 25 MW m ⁻² K ⁻¹	Steady-state Raman		[72]
	/multilayer h-BN				
	Local registry in multilayer Gr/h-BN	Registry dependent ITC with ABp > DW > AB > AA	NEMD	Change interlayer force constants and mode coupling	[144]
	Defective Gr/MoS ₂ heterobilayer	Increase ITC by 80% with 5% concentration of C-vacancy defect	AEMD	Reshape phonon spectral overlap	[173]
	Multilayer Gr/h-BN with atom diffusion	Composition diffusion can improve ITC by up to ~70%	NEMD	Modify phonon spectral overlap	[176]
	Functionalized Gr/h-BN heterointerface	NH ₂ functionalization enhances ITC by over 800%	NEMD	Strengthen vdW coupling	[177]
	Twisted MoS ₂ /WS ₂ heterobilayer	Interlayer twist enables a 2.5-fold increase in ITC	TDTR	Activates efficient phonon conversion through inelastic scattering	[13]
	Strained graphene Kirigami heterostructure	ITC can be continuously regulated by in-plane tensile strain	AEMD	Change interfacial interaction density and delocalized phonon-mode distribution	[184]
	MoS ₂ /organic interface	ITC is one order of magnitude lower than MoS ₂ single crystal	Laser Flash Method	Induce structural disorder and increased phonon scattering rate	[190]
	Gr/h-BN monolayer	4.3 GW m ⁻² K ⁻¹	NEMD	/	[198]
	Gr/BCN monolayer	4.9 GW m ⁻² K ⁻¹			
	Gr/BC ₂ N monolayer	4.0 GW m ⁻² K ⁻¹			
	Gr/h-BN monolayer with interface diffusion	Interface diffusion reduces TC of heterostructure	NEMD	Anderson localization of phonons	[66]
	Periodic MoS ₂ /MoSe ₂ array	Thermal conductivity is non-monotonic with period number	NEMD	Incoherent-to-coherent phonon crossover	[194]
	MoSe ₂ /WSe ₂ monolayer	TR ratio of 96% and can be regulated by rotating the angle of interface	H-type method	Asymmetric phonon spectral matching and localized phonon modes	[24]
	Gr/h-BN monolayer	TR ratio of ~170% and can be enhanced to 334% with chirality angle	NEMD	Direction-dependent asymmetry in mismatch of phonon density of states	[193]
	Gr/h-BN hybrid multilayer structure	Largest TR ratio of 280%	NEMD	Direction-dependent phonon scattering	[197]

2D: two-dimensional; ITC: interfacial thermal conductance; TC: thermal conductivity; vdW: van der Waals; BN: boron nitride; TDTR: time-domain thermoreflectance; NEMD: nonequilibrium molecular dynamics; AEMD: approach-to-equilibrium molecular dynamics.

5.2 From heat dissipation to thermal functionality

The significance of such control becomes clearest when interfacial heat transport is considered in the context of device operation. In

many atomically thin devices, heat generated by electrical bias, optical excitation, non-radiative relaxation, or local switching must cross one or more heterointerfaces before it can spread into the substrate or surrounding environment^[3,199]. When those interfaces are weakly transmitting, thermal energy accumulates near the active region, producing hot spots, spatially nonuniform operation, performance drift, and accelerated degradation^[10,200]. Similar bottleneck considerations also arise in layered thermal interface materials and inorganic/organic hybrid systems, where heat must pass across numerous filler-matrix interfaces before reaching an external heat sink^[201-204].

Yet to regard interfacial heat flow only as a parasitic limitation is to overlook its broader role in determining how a device actually operates. In 2D heterostructures, interfaces do not simply regulate how heat leaves a device. They also influence where temperature gradients form, how local heating couples back to charge transport or optical response, and whether an operating state remains stable under repeated biasing. Because the same interface that governs thermal dissipation often also defines the electronic or optoelectronic processes on which the device relies, interfacial thermal transport is more appropriately understood as part of device function rather than as an external constraint imposed upon it.

This coupling becomes especially important in emerging device architectures, including switching, memory, memristive, neuromorphic, and optoelectronic heterostructures^[3,205-207]. In such systems, local temperature rise can degrade mobility, shift threshold behavior, increase leakage, enhance hysteresis, and compromise endurance and operational reproducibility^[208-213]. At the same time, controlled local heating may also participate constructively in device operation by assisting ion motion, defect rearrangement, conductive-path evolution, phase or structural transitions, and interfacial recombination processes^[18,214,215]. The key point is that the most useful interface is not necessarily the one with the highest thermal conductance. Functional operation may instead require a balance between local thermal activation and efficient heat removal, so that the interface supports the desired device process without driving excessive thermal nonuniformity or instability.

Viewed from this perspective, interfacial heat transport becomes a natural entry point to thermal functional devices. Thermal diodes, switches, transistors, and broader phononic concepts have long provided the conceptual framework for controlling heat flow rather than merely dissipating it (Figure 5d)^[21-25,188,216]. What 2D heterostructures add is a uniquely accessible interface platform whose structure can be defined, tuned, and potentially coupled to external perturbation with unusual precision. This opens a route toward interfaces that do more than passively conduct heat: they may rectify heat flow, modulate it between distinct operating states, or couple thermal response to electrical or optical inputs. Even when such behavior is not used to build dedicated phononic devices, the same logic remains valuable at the level of conventional electronics. An interface whose thermal conductance can be deliberately suppressed, enhanced, or dynamically reconfigured could help redistribute heat away from vulnerable regions, confine it where activation is required, or stabilize device operation under nonuniform loading. In that sense, thermal functional behavior need not be confined to stand-alone thermal devices, but may instead become embedded within heterogeneous electronic and optoelectronic architectures.

5.3 Toward actively addressable thermal interfaces

The diversity of 2D heterointerfaces provides an unusually rich platform for controlling interfacial heat transport. Their significance lies not in optimizing ITC in a single direction, but in enabling it to be increased, reduced, or dynamically reconfigured according to the demands of a given application, whether the goal is rapid heat dissipation, local heat confinement, directional heat-flow control, or more complex thermal functionality. As 2D heterostructures move toward dense integration, multifunctional stacks, and heterogeneous circuits, local control of interfacial heat flow may become as important as the intrinsic thermal conductivity of the constituent layers themselves.

The most attractive future strategies will be those that achieve controllable and reversible modulation of interfacial heat transport in the simplest possible manner. In particular, tuning ITC directly through mechanical, electrical, magnetic, optical, or ionic signals is especially compelling, because it would allow the interface to evolve from a structurally defined boundary into an actively addressable thermal element. For such interfaces, the relevant figures of merit extend beyond the magnitude of conductance modulation. A useful interface must also retain its response over many cycles, remain thermally and chemically stable under bias or optical excitation, respond on timescales compatible with device operation, and be compatible with scalable fabrication. Ion-intercalation-based control may provide a large modulation window, but can be limited by slow kinetics, hysteresis, and cycling fatigue. Strain- or pressure-based control can directly modify interlayer coupling, but its integration into dense circuits remains challenging. Field-driven control could provide an attractive low-power route, although its influence on heat flow still requires direct operando verification. The central question is whether its thermal response can be matched to the function of the device it supports. This shift from passive heat removal to functional heat-flow control is likely to define the next stage of interfacial thermal engineering in 2D heterostructures.

6. Outlook

The next decade of interfacial thermal transport in 2D heterostructures will be shaped by a shift from characterization to design. As 2D electronic devices, optoelectronic systems and integrated circuits based on atomically thin materials advance rapidly, their

performance, reliability and scaling may increasingly be limited not only by intrinsic channel properties, but also by how efficiently heat crosses, accumulates or is redirected at interfaces. The central challenge is to turn the structural sensitivity of 2D heterointerfaces into predictive and controllable thermal response. Rather than treating ITC as a value measured after fabrication, future studies should define target thermal behaviors in advance and use growth, transfer, alignment, strain, substrate morphology and post-processing as tools for thermal materials design.

Progress will require structurally resolved design rules. Directly grown lateral junctions, transfer-assembled vdW stacks, periodic superlattices and reconstructed moiré systems each create distinct phonon landscapes, yet the field still lacks a quantitative map linking formation history to local spacing, registry, contact quality, defect structure and ITC. Establishing this connection will require correlative workflows in which thermal measurements are paired with structural, spectroscopic and microscopic characterization of the same interface. ITC should ultimately be assigned to a defined interfacial state rather than merely a material combination.

Equally important is the development of spatially resolved thermal physics. Many of the features that make 2D heterostructures thermally distinctive, including moiré domains, reconstructed boundaries, nanoscale wrinkles, trapped adsorbates and 1D channels, lie below the resolution of conventional thermal probes. Yet these local structures can dominate the measured response. Future metrology should move from single-point averages toward maps that connect local structure, local phonon behavior and local temperature fields. Raman and TDTR mapping methods, scanning-probe-assisted thermal metrology, vibrational STEM-EELS, ultrafast diffraction and hybrid optical-electrical approaches may together make it possible to interrogate interfacial heat flow at the length and time scales on which it is actually governed.

Another major frontier is dynamic and operando control. The most relevant interfaces in future devices will not be static. They may be strained, gated, charged, intercalated, optically excited or driven close to switching conditions. Measurements and models must capture how heat flow evolves under external actuation, rather than only comparing separate equilibrium states. The critical metrics will include modulation ratio, reversibility, response speed, fatigue resistance and compatibility with device operation. Only with these metrics can ITC be evaluated as a true device variable.

Predictive modelling will also need to become more mechanism-informed and structurally realistic. First-principles methods describe bonding, phonons and interfacial force constants with high fidelity, but remain limited in size and time. Molecular dynamics can access larger systems and directly include finite-temperature anharmonicity, disorder and registry-dependent configurations, although its accuracy is ultimately limited by the quality of the interatomic potential. Machine-learning interatomic potentials offer a promising route between these limits, especially for moiré supercells, disordered contacts and field-modulated structures. Their value will lie not simply in reproducing measured conductance, but in revealing which structural variables control elastic transmission, inelastic scattering, localized modes, rectification, and active modulation.

The ultimate design target should be application-specific thermal response. 2D devices will not benefit from a universal rule such as maximizing ITC. Logic and high-power devices may require rapid heat extraction; memory and switching elements may benefit from local thermal activation; optoelectronic heterostructures may demand temperature uniformity and spectral stability; thermal circuits may require rectification or switchable heat flow. Thermal transport should be considered alongside band alignment, carrier mobility, exciton dynamics, ferroelectricity, and mechanical compliance during device design.

Taken together, these directions can be summarized as five near-term priorities for the field (Table 3). They point toward a future in which 2D heterointerfaces are treated as programmable thermal matter, with interfacial heat flow structurally defined, spatially resolved, dynamically actuated, physically predicted and designed for device operation. If these capabilities mature together, interfacial heat transport will move from a parasitic constraint to an active design variable. This transition from passive thermal boundaries to addressable heat-flow elements is likely to become one of the defining opportunities for 2D heterostructure thermal science in the coming decade.

Table 3. Near-term priorities for 2D heterointerface thermal science.

No.	Future directions
1	Structure-defined conductance: Establish quantitative links between ITC and well-defined interfacial structures.
2	Spatially resolved thermal physics: Resolve how nanoscale heterogeneity shapes local heat flow.
3	Operando control: Measure tunable interfaces under realistic mechanical, electrical, optical or ionic driving.
4	Predictive modelling: Build models that connect experimentally realistic interfaces to phonon-level transport mechanisms.
5	Application-specific design: Define thermal responses that match the operating needs of future 2D devices.

2D: two-dimensional; ITC: interfacial thermal conductance.

Declarations

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Authors contribution

Zhang Y: Writing-original draft, writing-review & editing.

Fan A: Writing-review & editing.

Ma W: Writing-review & editing, supervision.

Zhang X: Conceptualization, writing-review & editing, funding acquisition, supervision.

Conflicts of interest

Xing Zhang is an Editorial Board Member, and Aoran Fan is a Youth Editorial Board Member of *Thermo-X*. The other authors declare no conflicts of interest.

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Not applicable.

Consent to participate

Not applicable.

Consent for publication

Not applicable.

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