

ACCEPTED MANUSCRIPT • OPEN ACCESS

Future of Condensed Matter Physics for the Next 10 Years

To cite this article before publication: Jonathan P Bird *et al* 2025 *J. Phys.: Condens. Matter* in press <https://doi.org/10.1088/1361-648X/ae0be1>

Manuscript version: Accepted Manuscript

Accepted Manuscript is “the version of the article accepted for publication including all changes made as a result of the peer review process, and which may also include the addition to the article by IOP Publishing of a header, an article ID, a cover sheet and/or an ‘Accepted Manuscript’ watermark, but excluding any other editing, typesetting or other changes made by IOP Publishing and/or its licensors”

This Accepted Manuscript is © 2025 The Author(s). Published by IOP Publishing Ltd.



As the Version of Record of this article is going to be / has been published on a gold open access basis under a CC BY 4.0 licence, this Accepted Manuscript is available for reuse under a CC BY 4.0 licence immediately.

Everyone is permitted to use all or part of the original content in this article, provided that they adhere to all the terms of the licence <https://creativecommons.org/licenses/by/4.0>

Although reasonable endeavours have been taken to obtain all necessary permissions from third parties to include their copyrighted content within this article, their full citation and copyright line may not be present in this Accepted Manuscript version. Before using any content from this article, please refer to the Version of Record on IOPscience once published for full citation and copyright details, as permissions may be required. All third party content is fully copyright protected and is not published on a gold open access basis under a CC BY licence, unless that is specifically stated in the figure caption in the Version of Record.

View the [article online](#) for updates and enhancements.

Future of Condensed Matter Physics for the Next 10 Years⁺

Jonathan Bird,¹ Jinguang Cheng,² Chun-Gang Duan,³ Thomas Frederiksen,^{4,5} Gerhard Kahl,⁶ Gianfranco Pacchioni,⁷ Je-Geun Park,⁸ Talat S. Rahman,⁹ Steven R. Schofield,¹⁰ Krishnendu Sengupta,¹¹ Xiaoshan Xu,¹² Jin Zhao,¹³ Peter A. Dowben^{12,*}

1) Department of Electrical Engineering, 230 Davis Hall, University at Buffalo, The State University of New York, Buffalo, NY 14260-1900 U.S.A; e-mail: jbird@buffalo.edu

2) Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China; e-mail: jgcheng@iphy.ac.cn

3) Key Laboratory of Polar Materials and Devices, School of Physics and Electronic Science, East China Normal University; Information Building, Room 224; 500 Dong-Chuan Rd., Shanghai 20024, China; e-mail: cgduan@clpm.ecnu.edu.cn

4) Donostia International Physics Center (DIPC), E-20018 Donostia-San Sebastián, Spain; e-mail: thomas_frederiksen@ehu.eus

5) IKERBASQUE, Basque Foundation for Science, E-48013 Bilbao, Spain; e-mail: thomas_frederiksen@ehu.eus

6) Institut für Theoretische Physik, Technische Universität Wien, Wiedner Hauptstrasse 8 - 10, A-1040 Wien, Austria; e-mail: gerhard.kahl@tuwien.ac.at

7) Dipartimento di Scienza dei Materiali, Università degli Studi di Milano-Bicocca, via R. Cozzi 55, 20125 Milano, Italy; e-mail: gianfranco.pacchioni@unimib.it

8) Department of Physics and Astronomy, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 08826, South Korea; e-mail: jgpark10@snu.ac.kr

9) Dept. of Physics, University of Central Florida, 4000 Central Florida Blvd. Building 121, Orlando, Florida 32816 U.S.A; e-mail: talat@ucf.edu

10) London Centre for Nanotechnology and Department of Physics and Astronomy, University College London (UCL), 17-19 Gordon Str., London WC1H 0AH, United Kingdom; e-mail: s.schofield@ucl.ac.uk

11) School of Physical Sciences, Indian Association for the Cultivation of Science, 2A and 2B Raja S.C. Mullick Road, Jadavpur, Kolkata-700032, West Bengal, India; e-mail: ksengupta1@gmail.com

12) Department of Physics and Astronomy, Theodore Jorgensen Hall, 855 North 16th Street University of Nebraska-Lincoln, Lincoln, NE 68588-0299 U.S.A.; e-mail: xiaoshan.xu@unl.edu, e mail: pdowben@unl.edu

13) University of Science & Technology of China, Teaching and Research Building B of
Material Science, Room B908, 96 Jinzhai Rd., Hefei, Anhui 230026, China; e-mail:
zhaojin4576@gmail.com

+) All authors contributed equally to this perspective

*) Author to whom correspondence should be addressed: pdowben1@unl.edu

keywords: condensed matter physics, magnetic ordering, ferroelectricity, superconductivity,
phononics, soft materials, nanoscale conductance, nonequilibrium, chemical physics

Abstract: This perspective outlines a selection of research directions that members of the JPCM editorial board anticipate may shape the frontier of condensed matter physics over the next decade. Rather than a comprehensive review or formal roadmap, this perspective reflects a set of informed views drawn from diverse areas of expertise. Our intention is to spark curiosity, provoke discussion, and encourage readers to imagine -- and pursue -- the exciting possibilities that lie ahead.

What might the next ten years hold for condensed matter physics? In this perspective, several section editors and editorial board members of the *Journal of Physics: Condensed Matter* and have drawn upon our collective expertise. Though by no means exhaustive, this perspective outlines topics we think may expand our understanding and which are coupled to questions that the community will likely investigate. Topics such as magnetic ordering, ferroelectric materials, superconductivity, non-equilibrium physics, phononics, soft materials, nanoscale conductance, symmetry breaking, chemical physics and advances in condensed matter theory are briefly touched upon but this is not intended to be a complete picture of the future of condensed matter physics, for the next 10 years as this is not a comprehensive review, nor a definitive roadmap. Instead, it reflects our shared sense of areas that could see significant development or yield unexpected breakthroughs. We hope it will serve as a springboard for discussion and imagination. As we have experienced in writing this article, thinking collectively about where our field is going has been a stimulating experience, and we invite readers to engage with the same sense of curiosity and possibility.

Magnetic ordering, spin currents and symmetry breaking:

The study of magnetism dates back millennia, but advances continue to keep the study of magnetism at the forefront of condensed matter physics. The field of magnetism is now undergoing another revolution on several fronts. There has been the identification of novel forms of chiral magnetism, including a ferromagnetic double helix [1], a variety of 3D chiral spin textures, such as helical spins [2] and skyrmion-like tube structures [3], with the latter two reported for FeGe alloys. This deepens our understanding of the vector spin exchange known as the Dzyaloshinskii–Moriya interaction, and its consequences. Recently, there has also been an increasing recognition of novel magnetic materials that are neither like colinear ferromagnets nor colinear antiferromagnets. Attracting much attention are the non-colinear antiferromagnets, now dubbed altermagnets. Altermagnets break time-reversal symmetry yet retain zero net magnetization despite exhibiting a spin-split band structure [4]. Rotation connects the opposite-spin sublattices but not translation nor inversion [4]. From angle- and spin-resolved photoemission, such altermagnetism has been recently identified in MnTe [5, 6]. Using angle-resolved photoemission in combination with angle-resolved magnetic circular and natural circular dichroism asymmetries has also been used to identify RuO₂ as an altermagnet [7]. It is worth noting that, without realizing, Shubnikov had already described, in the 1950's, the colored point groups of altermagnets [8] that allow one to classify altermagnets.

Chirality-induced spin selectivity has now been identified in inorganic chiral crystals Cr_{1/3}NbS₂ [9], transition-metal disilicides NbSi₂ and TaSi₂ [10], and chiral crystals of Te [11] leading to observations of current-induced magnetization in elemental tellurium [11] and chirality-induced spin currents [11-13]. While the loss of inversion symmetry will lead to spin-orbit coupling (SOC), as occurs in chiral systems, the systems with heavier elements are thought to have more spin-orbit coupling, thus interplay of chirality, spin-orbit coupling, and chirality-induced spin currents is very far from fully elucidated [14].

When interfacing organic materials with ferromagnets, there is a growing body of experiment to suggest that the paramagnetic correlation lengths in the organic film or material are large, perhaps of the order of many nanometers [15]. If this is ultimately verified, it will be unprecedented and would require a full theoretical explanation. But first an experiment must establish if the suggested large paramagnetic correlation lengths exist, as indicated in some organic materials. What is clear that organic chiral molecules [12,16-22], of a single enantiomer (left or

right handed), also exhibit chirality-induced spin selectivity. We envision that demonstrations of topologically protected spin current in organic chiral phototransistors may also be possible.

Magnetism in reduced dimensions, multiferroics and magneto-electric coupling:

It has been recognized that the magnetic Curie temperature has a dimensionality crossover, with decreasing magnetic film thickness, from 3-dimensional to 2-dimensional [23-25]. So how magnetism behaves in two dimensions has not only been one of the enduring questions in condensed matter physics, but understanding magnetism in reduced dimensionality has significance for our understanding of magnetism generally. Thus, the advent of van der Waals magnets has provided opportunities for new insights into questions regarding 2-dimensional magnetism and progress has been amazing, despite their relatively short history [25,26]. One area of development is the confirmation that intrinsically two-dimensional magnets can be profoundly different from bulk magnets and exhibit novel functionalities [27]. Another exciting development is the realization of novel quantum states using these materials, whether in the form of heterostructures or twisted systems [28]. Equally intriguing is the connection to fundamental quantum-mechanical concepts such as the quantum metric and Berry curvature [29]. How these quantum properties are revealed and realized in van der Waals magnets remains an open question and exciting avenue for research.

Two-dimensional magnetism can emerge exclusively from orbital degrees of freedom, bypassing conventional electron spin mechanisms [30,31]. The orbital motion simultaneously generates a novel ferroic order - the ferrovalley in which the spin-orbit coupling coexists with the intrinsic exchange interaction [32]. As an example, the ferromagnetic semiconductor VSe₂ monolayer is predicted to have potentially spontaneous valley polarization and chiral dependent optical excitations [32]. These dual ferroic orders share a common orbital origin, resulting in inherently strong ferroic couplings and large responses to external fields, endowing such two-dimensional multiferroic materials (materials with the coexistence of two or more ferroic orders) with potentially extraordinary multifunctional adaptability [33]. More generally, the ferrovalley is the spontaneous valley polarization, and is generally coupled with other ferroic orders, like ferromagnetism (spin polarization) or ferroelectricity (charge polarization). Much work remains to be done both for fundamental understanding of the ensuing mechanisms and the attainment of practical applications.

The use of on-surface synthesis to fabricate open-shell nano-graphenes with atomic precision has enabled the long-anticipated emergence of π -magnetism to be experimentally realized, providing a versatile platform for exploring localized spin states, magnetic exchange interactions, and strong electron correlations at the atomic scale [34]. The evolution of synthetic routes to stabilize larger and more complex open-shell structures might provide the setting for optimal quantum coherence and manipulation, as well as to scale up these systems to form controllable quantum spin lattices. These advances may also provide unprecedented opportunities for research in low-dimensional multiferroics in which the coupling mechanisms among ferroic orders, strong electronic correlations, and emergent topological states in orbital-derived multiferroics constitute both challenges and opportunities for condensed matter physics in the coming decade. The unique interplay of symmetry-breaking orbital textures and quantum geometric effects in these systems is poised to redefine fundamental paradigms in quantum material design while pushing the boundaries of non-volatile memory and neuromorphic computing technologies. These systems are now central to efforts at realizing highly entangled quantum spin states, with potential applications in spintronics and quantum information science. Their flexibility and controllability place them

within the broader context of an emerging quantum-coherent nanoscience, where coherence and interaction effects are engineered at the nanoscale [35].

If we look at much broader impacts, there is an ever-wider recognition that the growth of logic and memory results in unsustainable increases in energy consumption [36]. A recent paper on this topic stated, "One promising type of energy efficient logic devices in research is based on the use of magnetoelectric (ME) materials." [37] Not surprisingly, an increasing number of device schemes have been discussed and various magnetoelectric devices have also been demonstrated [38]. Yet, a great deal of physics remains to be fully established, despite the growing attention given to this topic. For magneto-electric devices based on magneto-electric antiferromagnets, there is an open question of what limits the antiferromagnetic domain switching speed [39]. While antiferromagnetic switching is widely touted to be faster than ferromagnetic switching, a better understanding and better characterization of switching mechanism is important. There is also much yet to be understood about the applicable scaling arguments, as this would not only affect switching speed, but would limit how small a device could be made, as well as determine the limits to the possible reduction of the coercive voltage.

Recent work, investigating the Néel vector orientation, has brought some novel new insights to light. Antiferromagnets are now seen to have a thermally fluctuating Néel vector independent of the crystal symmetry [40]. There are also demonstrations that the Néel vector under an applied voltage that deviates from the polar axis of the boron doped antiferromagnet $\text{Cr}_2\text{O}_3(0001)$ [41]. The diminished role of the expected antiferromagnetic magneto-crystalline anisotropy remains puzzling and needs to be fully explained.

Superconductivity:

Nickel-based oxides (nickelates) have emerged as a new family of superconductors with unconventional high- T_c superconductivity. With Ni being the nearest neighbor of copper in the periodic table of elements, the quest of nickelate superconductors began soon after the discovery of the cuprate high- T_c superconductors. Eventually, $\text{Nd}_{1-x}\text{Sr}_x\text{NiO}_2$ thin films were found to be superconducting ($T_c \approx 9\text{-}15\text{ K}$), with infinite-layer structure [42]. The family of nickelate superconductors quickly expanded to include the bilayer and trilayer Ruddlesden-Popper phases of the form $\text{R}_{n+1}\text{Ni}_n\text{O}_{3n+1}$ ($n = 2, 3$) [43,44], as well as the hybrid Ruddlesden-Popper phase $\text{La}_5\text{Ni}_3\text{O}_{11}$ [45]. This in turn led to the discovery of non-cuprate unconventional superconductor surpassing the boiling point of liquid nitrogen, i.e., the bilayer $\text{La}_3\text{Ni}_2\text{O}_7$ with $T_c \sim 80\text{ K}$ under about 14 GPa [43]. Very recently, ambient-pressure superconductivity, with T_c^{onset} over 40 K, has been successively realized in bilayer nickelate $(\text{La,Pr})_3\text{Ni}_2\text{O}_7$ thin films, stabilized via in-plane compressive strain and ozone post-annealing process [46-48]. Yet further optimization of the nickelates is needed in order to achieve similar high T_c values as seen in the pressurized nickelate bulk samples. Despite encouraging progress, there remain critical questions to be addressed in this field. For example, both the infinite-layer and Ruddlesden-Popper nickelates suffer from sample quality problems and the latter are prone to intergrowth of different Ruddlesden-Popper phases while oxygen vacancies lead to complications [49,50]. In addition, unlike the single-band model for the cuprates superconductors, both e_g orbitals, i.e. the d_{z^2} and $d_{x^2-y^2}$, should play an important role in governing high- T_c superconductivity. In the absence of consensus, more in-depth investigations are needed to reveal the superconducting mechanism(s).

Broken inversion symmetry is a critical feature of materials, not only intrinsic to magnetism (as discussed above), ferroelectric properties, but also may affect superconductivity. Chiral superconductors may emerge in novel topological materials in which the superconducting

states break time reversal symmetry or inversion symmetry [51]. Although uncommon, recent work on non-oxide 2D heterolayers may have now given us a more convincing example of chiral superconductors [52] beyond metals like LaPt_3P [53] and Sr_2RuO_4 [54]. One approach to achieving chiral superconductors is by introducing the moiré superlattice between adjacent graphene or graphene and h-BN layers [55-58]. Convincing proof of chiral superconductivity remains challenging, with perhaps the most compelling proof, to date, recently shown in rhombohedral graphene [59], with a T_c of 300 mK. Despite the challenges, chiral superconductors, while extremely fragile, may be the key to identifying the presence of Majorana zero modes [51]. Majorana bound states are specific examples of non-Abelian anyons [60] which are quasiparticles that do not follow typical fermionic or bosonic statistics and, so far, have been quite elusive [61-63]. The anyon, or quasiparticles that exist in 2 (or lower) dimensions with statistics between fermions and bosons was, we note in passing, originally discussed and named by Frank Wilczek in 1982 [64], and reviewed in a "Physics World" perspective later [65].

The interplay between magnetism and superconductivity remains a rich area of study. Scanning tunneling microscopy (STM) enables the creation and probing of Yu-Shiba-Rusinov (YSR) states, which arise from the interaction of magnetic impurities with a superconducting condensate [66]. This atomic-scale control underpins research efforts to realize topologically non-trivial superconducting states hosting Majorana modes [67], as well as broader explorations of topological superconductivity in artificial spin lattices [68]. Advances in atomic-scale fabrication and theoretical modelling are expected to deliver transformative insights into topological phases of matter. One goal that could result from a synergy of characterization techniques would be a compelling demonstration of Majorana modes.

Ferroelectricity:

If broken inversion symmetry causes a switchable spontaneous polarization, one has a ferroelectric material. For this reason, the discovery of new ferroelectric materials is always exciting. Among the novel ferroelectric materials, orthorhombic hafnia, which was discovered a little more than a decade ago, stands out because of its CMOS compatibility (basically with possible implementation consistent with current silicon memory chip manufacturing) [69]. Its uniqueness as a condensed matter system was later realized in that the unit cell of ferroelectric hafnia, HfO_2 , consists of both a non-polar layer and a polar layer. The hafnia ferroelectric polarization reversal comes from in-layer displacement of oxygen atoms [70]. This weakens the interaction between dipoles of neighbouring polar layers, causing the so-called flat phonon bands and polarization switching that is nearly independent of film thickness and domain size (down to the single unit cell) thus "scale-free" ferroelectricity [71]. Moreover, negative domain-wall formation energy was revealed, suggesting that the polarization in neighbouring polar layers tends to be antiparallel. Hence, orthorhombic hafnia might be close to a model antiferroelectric system, with a ferroelectric metastable state that resembles Kittel's proposal [72]. The next 10 years may very well see more in-depth exploration of the ferroelectricity in orthorhombic hafnia down to the two-dimensional limit, the role of oxygen displacement, as well as its antiferroelectricity, which is much needed for energy storage applications. Ferroelectric behavior in 2 dimensions, already seen some time ago in organic ferroelectrics [73], might well be expanded to 2D multiferroics [74].

Establishing a link to neighboring fields [74], we also need to mention the development and the understanding of ferroelectric liquid crystals which will likely be of major interest in the near future. Indeed, there is now some recognition that the long-sought [75] and recently

demonstrated ferroelectric nematic liquid crystals [76] can adopt chiral ground states, even when made from achiral molecules [77].

Nanoscale conductance:

Not only is there recognition of dimensionality-driven magnetic behaviour, but scaling effects are also now seen with the nonmetal-to-metal transition and conductance. For example, $\text{SrIrO}_3(001)$ exhibits a film-thickness-driven metal-insulator transition [78-80]. As wires become smaller and smaller, are Cu, Ag and Au still the best conductors? While Cu is generally considered one of the very best conductors ($1.68 \mu\Omega \text{ cm}$), the resistance of Cu wires becomes less appealing at wire widths on the nanometer scale because of grain boundary and surface scattering. There is promise in the quasi-one dimensional trichalcogenide wires of TaSe_3 [81] and ZrTe_3 [82] that may well do better at wire widths of a few nanometers. These quasi-one-dimensional materials surpass Cu for very narrow wires because of diminished edge scattering, even though the conductivity of bulk Cu, Ag and Au is higher. The effect of temperature makes a comparison between these quasi-one-dimensional material and the better known conductors even more complex as resistance changes due to a charge density wave (at about 63 K for bulk ZrTe_3 [83-86]) and superconductivity, which can set in at much lower temperatures in the region of 2 K [85-87]. Making the physics even richer, the periodic lattice distortion can be incommensurate [88]. So, the effect of dimensionality (in this case wire widths) remains far from fully explored.

Phononics and nonequilibrium:

Another important topic is quantum phononics [89-96], which promises to develop the next-generation techniques for single-phonon manipulation and detection. If realized, these breakthroughs may rival those single particle techniques that have long existed for electrons and photons. The field of quantum phononics seeks to move on from the concept of the uncontrolled phonon bath as a source of decoherence, to develop techniques in which phonons can be generated, transmitted and detected at the level of countable numbers of quanta. There are also fundamental questions to address, as quantum phononics also involves the need to engineer phononic coupling to the environment via suitable materials choice and structural design. In addition to basic interest in this problem from a perspective of fundamental, solid-state physics, the potential applications are broad, including quantum sensing [93], quantum computing [94,97] and quantum communications [89,91,95,96]. Experimental examples, pointing to the potential applications abound, as in the recent demonstration of inelastic tunneling creating phonon emission at a defect [98]. Chiral phonons [99,100], as occur in systems with threefold rotational symmetry, imparting a quantized pseudo angular momentum, may induce spin polarization in a nonmagnetic electronic structure [101,102].

Nonequilibrium dynamics in quantum systems has gathered tremendous momentum over the last couple of decades. Initial work in this area involved study of situations where a parameter of the Hamiltonian describing a quantum system is changed suddenly (quench) or at a fixed rate (ramp) from an initial to a final value. The more recent studies of nonequilibrium dynamics in quantum mechanics have mostly focused on periodically driven systems [103-109]. The dynamics of such periodically driven systems at times which are integer multiple of drive periods, are described by their Floquet Hamiltonians. Typically, such driven systems heat up to an infinite temperature steady state [110]. At high frequencies or amplitudes, the systems, however, tend to show a variety of phenomena such as dynamical freezing, dynamical localization, realization of time crystalline state of matter and generation of topological states [103-109] at an intermediate,

prethermal, timescale. These phenomena do not have an analogue in either equilibrium or for systems subjected to aperiodic or random drives. Indeed, many of these phenomena may be tied to the presence of an approximate emergent symmetry of the Floquet Hamiltonian that controls the dynamics of such systems occupying a large pre-thermal timescale [109]. Ultracold atom systems, being sufficiently decoupled from the environment, serve as an important experimental platform for such dynamical phenomena [111]. A long-standing problem in nonequilibrium systems has concerned the nature of the field-induced breakdown of insulating behavior in correlated materials such as charge-density wave systems. Driven by an electric field, or thermal effects, quantum mechanical processes can result in a cascade-like or quantum avalanche transition from an insulating to a conducting state [112]. Recent theoretical advances [112], invoking the role of “quantum avalanching” to account for this behavior, provide a new direction for interpreting the behavior of quantum systems far-from-equilibrium. Highlighting the role of virtual phonon processes in the excitation of transport, this work also demonstrates how transport under nonequilibrium may differ profoundly from that in the linear (weak bias) regime.

Several theoretical challenges remain in this field. For example, the concept of universality and renormalization group, which has been central to quantum systems in equilibrium, is not fully understood for either closed or open driven quantum systems. Seeking a uniform theoretical framework for understanding universality and finding a possible classification of universal features that may arise in such systems constitute important theoretical problems [113]. In addition, there are theoretical challenges that emerge when one tries to understand periodically driven open quantum systems, i.e. quantum systems connected to an external bath. There are approaches to understanding effect of a bath on a non-driven quantum system through Lindblad operators but, for driven systems, the issue of existence of such Lindblad operators is still in question [114]. Thus, a general understanding of the nature of the steady states of periodically driven open quantum systems is still lacking. As an aside, the ramp dynamics of driven quantum systems, through a quantum critical point, showed universal power-law behavior, termed as Kibble-Zurek scaling, for excitation density and absorbed energies [115-119], and we note that Tom Kibble (of Kibble-Zurek scaling) and Ajit Srivastava edited a special issue for JPCM on “Condensed matter analogues of cosmology” [120].”

Time-resolved spectroscopies and physics at the ultrafast time scale:

In recent decades, time-resolved ultrafast laser techniques, based on pump-probe technology, have been combined with various experimental methods in condensed matter physics, leading to the development of time-resolved absorption and photoemission spectroscopy [121, 122], time-resolved angle-resolved photoemission spectroscopy (TR-ARPES) [123-125], ultrafast scanning tunneling microscopy (ultrafast STM) [126], ultrafast electron diffraction (UED) [127]. Focusing laser pulses in the THz range onto the STM tunnel junction generates transient bias pulses with femtosecond temporal resolution, enabling the tracking of intrinsic dynamics in single molecules [128] and the probing of defect states in two-dimensional materials on timescales faster than lattice vibrations [68]. These methods combine atomic spatial resolution with sub-picosecond temporal and millielectronvolt energy resolution. STM-based optical techniques, like scanning tunnelling luminescence and tip-enhanced photoluminescence, enable direct measurement of optoelectronic properties of single molecules and defects, including single-photon emitters with relevance to quantum technologies [129]. All of this has opened the door to investigation of ultrafast excited state dynamics in condensed matter systems, such as lattice, electrons, and spins.

As new experimental techniques become available, understanding the physical picture of the ultrafast dynamics has required developing real-time first-principles methods. Recently, real-time dynamical methods have gradually been adopted to study such problems. Excited-state dynamics can be divided into two parts: the photoexcitation and the relaxation. For the photoexcitation process, the crucial point is to describe the light-matter interaction. Various methods have been developed, such as the time-dependent Schrödinger equation (TDSE) [130], the semiconductor Bloch equations (SBE) [130], real-time Time-dependent Density Functional Theory (rt-TDDFT) [131-134]. Time-dependent Bethe-Salpeter Equation (TDBSE) [136], time-dependent adiabatic GW, Green's function (TD-aGW) methods [137], and density matrix based TDDFT [138,139]. For systems in which electron correlations are significant, a methodology that combines Dynamical Mean Field Theory (DMFT) with TDDFT [140-141] has been proposed. These methods enable the study of the dynamics of charge carriers excited by light, nonlinear optical effects, and the many-body effects of electron-hole pairs forming excitons during the excitation processes. Based on the Boltzmann transport equation, the real-time Boltzmann Transport Equation (rt-BTE) method has been developed to study carrier relaxation dominated by electron-phonon coupling within the quasi-classical approximation [142]. Beyond the quasi-classical approximation, and closer to "quantum dynamics," are methods that incorporate non-adiabatic effects. Currently, two main approaches have been developed that include non-adiabatic effects: one involves combining of rt-TDDFT with Ehrenfest dynamics, to study the dynamics of the coupled lattice and electrons together in the mean-field potential surface [131-135]. The other approach involves combining the time-dependent Kohn-Sham equation (TDKS) with the surface-hopping method, introducing a classical path approximation (CPA) [143]. Non-adiabatic molecular dynamics (NAMD) is based on the classical path approximation. Moreover, the various theoretical framework can be combined with different levels of electronic structure methods. For example, combining with spin-orbit coupling can be used to study spin dynamics [144]; combining with the GW + BSE method (GW + real-time BSE) can be used to study exciton relaxation [145]; and directly introducing the electron-phonon coupling matrix into the Hamiltonian allows for studying charge carrier dynamics in momentum space (NAMD_k) [146]. NAMD codes, such as Hefei-NAMD and Pyxaid, are increasingly being applied to condensed matter systems [143,147] broadening our understanding of ultrafast excited state dynamics in condensed matter systems. At the same time exciton-phonon interactions appear to compete with electron-phonon interactions in controlling the binding energy and lifetime of excitons in two-dimensional transitional metal dichalcogenides [139]. Yet, in the field of first-principles calculations, theoretical methods to study the excited-state dynamics of electrons, holes, spins, excitons, and other carriers are still in their early stages. We expect to see important developments in these areas driven by improved methodologies and increasing computational capabilities. Further developments in these theoretical and computational techniques should enable direct comparison with the multitude of pump-probe measurements using a variety of time and angle-resolved spectroscopic technique that document structural and electronic evolution of low dimensional systems far from equilibrium.

Density functional theory-based machine learned approaches:

In recent years, condensed matter physics has witnessed a paradigm shift from traditional density functional theory (DFT) calculations to machine learning (ML) driven approaches, revolutionizing material property predictions [148]. While DFT plays a foundational role for much of condensed matter theory, in part because of the quantum-scale accuracy, there are difficulties in apply DFT to very large systems. Although increasingly larger systems are now accessible to

DFT, ML models trained on DFT datasets now bridge the gap between the size scale typical of DFT and much greater length scales, enabling efficient simulations at mesoscopic or even macroscopic scales. State-of-the-art implementations, including graph-based neural networks and equivariant architectures, demonstrate remarkable successes possible in predicting phase transitions [149], electronic structure [150], mechanical responses [151], and high-order tensor properties [152]. Machine-learning driven approaches are a route to achieving near-DFT accuracy while operating at time and space scales inaccessible to traditional quantum simulations. This methodological advancement enables the exploration of complex systems with atomic-level resolution across experimentally accessible scales, thereby bridging the gap between quantum-mechanical precision and mesoscopic/macroscopic material behavior. The synergistic integration of physics-informed neural architectures with scalable data-driven frameworks is expected to facilitate the accelerated discovery of emergent phenomena in larger-scale systems such as twisted moiré superlattices and designer metamaterials in the near future.

There are other applications for machine learning (ML) derived potentials for DFT calculations. There is increasing evidence that in most cases the structure of a catalyst is not static but changes dynamically with the external conditions of temperature, pressure, etc. Catalytic activity as ferroelectric surfaces can differ at ferroelectric domain walls and on polarization, thus can be voltage controlled. Modeling these various complexities is presently out of reach of *ab initio* molecular dynamics (MD) simulations, but in developing accurate machine learning potential may lead to descriptions of dynamical phenomena and in particular structural evolution during heterogeneous catalysis reactions [153]. One open challenge, however, is to include long-range interactions in these ML-potentials, which is likely to become a focus area.

In parallel, tensor-network methods, especially the density matrix renormalization group (DMRG) and matrix product states (MPS), have become indispensable for simulating low-dimensional strongly correlated systems [154]. These methods have revealed a rich landscape of many-body phenomena, including the interplay between antiferromagnetic interactions, geometric frustration, and topological order in quantum magnets. Recent developments such as projected entangled pair states (PEPS) and infinite PEPS (iPEPS) have extended these capabilities into two dimensions. Beyond classical simulation, tensor networks are increasingly informing quantum algorithm design, for example through variational ansätze inspired by MPS and PEPS structures and serve as key benchmarks for near-term quantum simulation experiments. We envision that such hybrid classical-quantum algorithms may become a scalable route to simulating strongly correlated materials and accelerate progress toward practical quantum simulation on noisy intermediate-scale quantum (NISQ) devices.

Chemical Physics:

Better understanding of chemical bonding, catalysis and the mechanisms for chemical reactions have been aided by advances in theory as well as vast improvements in molecular imaging. Atomic force microscopy (AFM) can achieve higher spatial resolution than scanning tunneling microscopy (STM), particularly when employing chemically functionalized tips (e.g., CO-terminated). This has enabled images of individual molecules offering a rare visual connection to the atomic world [155]. The identification of increasingly complex molecules and improved chemical sensitivity is anticipated over the next decade [156]. Complementary advances in on-surface synthesis are allowing access to elusive molecular structures through thermal, optical, or tip-induced reactions. This opens pathways to engineered molecular systems with high-spin ground states, artificial spin lattices [157],

topologically non-trivial properties, and increasingly sophisticated molecular machines. Many opportunities remain in extending these studies to new substrates and integrating complementary techniques such as inelastic electron tunnelling spectroscopy (IETS), as noted above, and electron spin resonance (ESR) [158].

Solid surfaces will continue to be the playground for the creation of nanoscale materials through either supramolecular overlayer formation or simply the formation of hybrid interfaces whether it is metal-semiconductor or organic-inorganic or some other variation. These reduced dimensional systems typically display electronic states that are distinct from the bulk and are responsible for properties such as catalytic activity, novel growth modes, and quantum confinement. There continues to be interest in inducing novel quantum properties by reducing the dimensionality of the surface electrons, as has been the case with molecular overlayers manipulating the characteristics of the “quasi” free two-dimensional electron gas present at the (111) surfaces of noble metals, leading to tunable artificial lattices, molecular nanogratings, or quantum dot arrays [159]. It has long been recognized that the surface state of Cu(111), Ag(111) and Au(111) can influence molecular adsorbate packing [160,161]. Indeed, perturbations to the free electron density at the surface are compatible with the much older concept of the 'through metal bond'. A recent focus is on engineering quantum states in artificial electronic Kagome lattices that may appear through an intricate interaction of molecular overlayers with surface states on metals such as Au and Cu [162].

Another area of growing interest may be the exploitation of metallic surface states of topological materials for chemical reactions such as water splitting, the oxygen evolution reaction (OER), the hydrogen evolution reaction (HER), etc. [163]. The idea is appealing as the topologically protected states in these materials provide a stable electron reservoir with high electronic conductivity and carrier mobility and well-defined spin states. In electrocatalytic water splitting, for example, control of the electron spin through chirality and magnetization using topological chiral semimetals (RhSi, RhSn and RhBiS) has helped overcome the sluggish kinetics of the anodic oxygen evolution reaction owing to the spin-dependent electron transfer process [164]. There is, however, the need to carry out fundamental studies of the physical and chemical properties of these intriguing quantum materials before we can fully understand the role of spin and chirality in facilitating chemical reactions. Development of computation techniques beyond single reference DFT, as afforded by multi-reference wave-function-based methods [165] may provide better description of electron correlations and spin characteristics of these and other hybrid systems involving organic-inorganic interfaces.

Soft matter, biophysics, liquids and organic electronics:

Expanding on progress in the highly active research fields of soft matter, biophysics, and liquids, the tremendous technical advances now allow experimentalists to manipulate and to observe single molecules. Yet, fundamental challenges to understand and to classify the observed out-of-equilibrium properties of these systems remain. A challenge is to push forward the design of smart models (theory and simulation) and the synthesis of smart micro-particles or of active matter systems, inspired by real particles, where “smart” refers to clusters or particles able to respond to their environment in order to adapt properties and shape to their surrounding.

A particular challenge will arise in this field from the extremely broad range of scales that extends from the microscopic level to macroscopic scales. Tremendous progress in novel techniques allow observation, manipulation and investigation of particles and fluids at the smallest scale, where microscopic interaction effects become relevant. To cope with the disparity in scales,

new techniques have to be developed in experiment, theory and simulation in an effort to understand – starting from the microscopic level – macroscopic properties. Increasingly complex functionalities of microscopic units (and their related models) could then lead to unusual properties of the macroscopic system. This route can, alternatively, also be realized in the inverse direction (“inverse design”) which lead to highly complex microscopic entities ([bio-]molecules, colloids, etc.) which then may self-ensemble into macroscopic systems with desired, targeted properties. We foresee such progress in this arena in the coming years.

Recently, organic electronic materials have seen increased recognition, partly driven by the demonstration of nonvolatile voltage-controlled switching of the spin state that appears to be correlated to abrupt changes in thin film conductance [166], by combining spin crossover molecular films with ferroelectric thin films. These transistor devices might be competitive with silicon technology if their resistance can be lowered, as they are demonstrated to work at room temperature and above. Yet the origin of the conductance, given that most spin crossover complexes have a large highest occupied to lowest unoccupied molecular orbital gap and why there is a conductance change with changing spin state remains elusive. Likewise, organic ambipolar transistors, when first suggested [167] attracted a lot of attention, but those papers then had to be retracted [167,168], resulting in considerable uncertainty. Finally, with the increasing number of demonstrations of verifiable working organic ambipolar transistors [169], some resolution to the potential of organic ambipolar transistors now has much more firm ground. Yet again, the origin of the conductance, for both electrons and holes in these systems is not fully explained. Nor is there much understood as to what may limit switching speed, as most experiments have depended on fast optical probes, rather than voltage. Given the fact that there is little theory addressing these questions, such systems seem ripe for future exploration.

In Summary:

It is clear that a lot of emerging condensed matter physics is driven by symmetry (breaking of inversion symmetry, presence of chirality, etc.) as well as improved techniques, both experimental and theoretical. Chirality and symmetry breaking, for example, can play a crucial role in magnetism, spin selectivity, superconductivity and there is now reason to believe that chiral phonons exist as well. Dimensionality and interfaces, both of long-standing interest in condensed matter, continue to play an important role in emerging condensed matter physics. The reader is reminded that this perspective, by necessity, is incomplete. Yet it remains our hope that we’ve highlighted some exciting avenues where we expect much progress in the coming 10 years. We hope to see more discussion regarding the future prospects in chemical physics, more discussion of the varied ongoing research in soft matter, a deeper dive into momentum microscopy implementation of time and angle-resolved photoemission, a much-expanded discussion of machine learning while making more of the links between physics and biology, materials science, in the future. Correctly mapping the changing face of condensed matter, however, can only be done looking backwards, and this is forward looking.

References

- [1] Sanz-Hernández D, Hierro-Rodriguez A, Donnelly C, Pablo-Navarro J, Sorrentino A, Pereiro E, Magén C, McVitie S, De Teresa JM, Ferrer S, Fischer P, Fernández-Pacheco A, 2020, "Artificial Double-Helix for Geometrical Control of Magnetic Chirality", *ACS Nano* **14**, 8084–8092.
- [2] Streubel R, Bouma DS, Bruni F, Chen X, Ercius P, Ciston J, N'Diaye AT, Roy S, Kevan

- SD, Fischer P, Hellman F, 2021, "Chiral Spin Textures in Amorphous Iron–Germanium Thick Films", *Adv. Mater.* **33**, 2004830.
- [3] Wolf D, Schneider S, Rößler UK, Kovács A, Schmidt M, Dunin-Borkowski RE, Büchner B, Rellinghaus B, Lubk A, 2022, "Unveiling the three-dimensional magnetic texture of skyrmion tubes", *Nature Nanotechnol.* **17**, 250–255.
- [4] Šmejkal L, Sinova J, Jungwirth T, 2022, "Beyond Conventional Ferromagnetism and Antiferromagnetism: A Phase with Nonrelativistic Spin and Crystal Rotation Symmetry", *Phys. Rev. X* **12**, 031042.
- [5] Krempaský J, Šmejkal L, D'Souza SW, Hajlaoui M, Springholz G, Uhlířová K, Alarab F, Constantinou PC, Strocov V, Usanov D, Pudenko WR, González-Hernández R, Birk Hellenes A, Jansa Z, Reichlová H, Šobán Z, Gonzalez Betancourt RD, Wadley P, Sinova J, Kriegner D, Minár J, Dil JH, Jungwirth T, 2024, "Altermagnetic lifting of Kramers spin degeneracy", *Nature* **626**, 517–522.
- [6] Lee S, Lee S, Jung S, Jung J, Kim D, Lee Y, Seok B, Kim J, Park BG, Šmejkal L, Kang CJ, Kim C, 2024, "Broken Kramers Degeneracy in Altermagnetic MnTe", *Phys. Rev. Lett.* **132**, 036702.
- [7] Fedchenko O, Minár J, Akashdeep A, D'Souza SW, Vasilyev D, Tkach O, Odenbreit L, Nguyen Q, Kutnyakhov D, Wind N, Wenthaus L, Scholz M, Rossnagel K, Hoesch M, Aeschlimann M, Stadtmüller B, Kläui M, Schönhense G, Jungwirth T, Hellenes AB, Jakob G, Šmejkal L, Sinova J, Elmers HJ, 2024, "Observation of time-reversal symmetry breaking in the band structure of altermagnetic RuO₂", *Sci. Adv.* **10**, eadj4883.
- [8] Shubnikov A V., Belov N V., 1964, *Colored Symmetry*. Pergamon Press (New York)
- [9] Inui A, Aoki R, Nishiue Y, Shiota K, Kousaka Y, Shishido H, Hirobe D, Suda M, Ohe JI, Kishine JI, Yamamoto HM, Togawa Y, 2020, "Chirality-Induced Spin-Polarized State of a Chiral Crystal CrNb₃S₆", *Phys. Rev. Lett.* **124**, 166602.
- [10] Shiota K, Inui A, Hosaka Y, Amano R, Ōnuki Y, Hedo M, Nakama T, Hirobe D, Ohe JI, Kishine JI, Yamamoto HM, Shishido H, Togawa Y, 2021, "Chirality-Induced Spin Polarization over Macroscopic Distances in Chiral Disilicide Crystals", *Phys. Rev. Lett.* **127**, 126602.
- [11] Furukawa T, Shimokawa Y, Kobayashi K, Itou T, 2017, "Observation of current-induced bulk magnetization in elemental tellurium", *Nat Commun* **8**, 954.
- [12] Waldeck DH, 2012, "Chiral-Induced Spin Selectivity Effect", *J. Phys. Chem. Lett.* **3**, 2178–2187.
- [13] Hirakida R, Fujimoto J, Ogata M, 2022, "Chirality-dependent second-order spin current in systems with time-reversal symmetry", *Phys. Rev. B* **106**, 085127.
- [14] Fujimori A, 2024, "When and how can structural chirality and electron spin be coupled?", *Journal Club J. Condens. Matter. Phys.* 6–9.
- [15] Chin WK, Tamang B, Zaz MZ, Subedi A, Viswan G, N'Diaye AT, Lai RY, Dowben PA, 2024 "Evidence of cooperative effects for the Fe(phen)₂(NCS)₂ spin crossover molecular complex in polyaniline plus iron magnetite", *Molecules* **29** 4574
- [16] Banerjee-Ghosh K, Dor O Ben, Tassinari F, Capua E, Yochelis S, Capua A, Yang SH, Parkin SSP, Sarkar S, Kronik L, Baczewski LT, Naaman R, Paltiel Y, 2018, "Separation of enantiomers by their enantiospecific interaction with achiral magnetic substrates", *Science* **360**, 1331–1334.
- [17] Ozturk SF, Liu Z, Sutherland JD, Sassellov DD, 2023, "Origin of biological homochirality by crystallization of an RNA precursor on a magnetic surface", *Sci. Adv.* **9**, eadg8274.

- [18] Liu T, Wang X, Wang H, Shi G, Gao F, Feng H, Deng H, Hu L, Lochner E, Schlottmann P, Von Molnár S, Li Y, Zhao J, Xiong P, 2020, "Linear and nonlinear two-terminal spin-valve effect from chirality-induced spin selectivity", *ACS Nano* **14**, 15983–15991.
- [19] Göhler B, Hamelbeck V, Markus TZ, Kettner M, Hanne GF, Vager Z, Naaman R, Zacharias H, 2011, "Spin selectivity in electron transmission through self-assembled monolayers of double-stranded DNA", *Science* **331**, 894–897.
- [20] Xie Z, Markus TZ, Cohen SR, Vager Z, Gutierrez R, Naaman R, 2011, "Spin specific electron conduction through DNA oligomers", *Nano Lett.* **11**, 4652–4655.
- [21] Dor O Ben, Yochelis S, Mathew SP, Naaman R, Paltiel Y, 2013, "A chiral-based magnetic memory device without a permanent magnet", *Nature Commun.* **4**, 2256.
- [22] Ben Dor O, Yochelis S, Radko A, Vankayala K, Capua E, Capua A, Yang SH, Baczewski LT, Parkin SSP, Naaman R, Paltiel Y, 2017, "Magnetization switching in ferromagnets by adsorbed chiral molecules without current or external magnetic field", *Nature Commun.* **8**, 14567.
- [23] Li Y, Baberschke K, 1992, "Dimensional crossover in ultrathin Ni(111) films on W(110)", *Phys. Rev. Lett.* **68**, 1208–1211.
- [24] Bramfeld TS, Willis RF, 2008, "Temperature-dependent crossover of dimensionality in ultrathin nickel films", *J. Appl. Phys.* **103**, 07C718.
- [25] Park JG, 2016, "Opportunities and challenges of 2D magnetic van der Waals materials: Magnetic graphene?", *J. Phys. Condens. Matter* **28**, 301001.
- [26] Burch KS, Mandrus D, Park JG, 2018, "Magnetism in two-dimensional van der Waals materials", *Nature* **563**, 47–52.
- [27] Gibertini M, Koperski M, Morpurgo AF, Novoselov KS, 2019, "Magnetic 2D materials and heterostructures", *Nature Nanotechnol.* **14**, 408–419.
- [28] Song T, Sun QC, Anderson E, Wang C, Qian J, Taniguchi T, Watanabe K, McGuire MA, Stöhr R, Xiao D, Cao T, Wrachtrup J, Xu X, 2021, "Direct visualization of magnetic domains and moiré magnetism in twisted 2D magnets", *Science* **374**, 1140–1144.
- [29] Yu J, Bernevig BA, Queiroz R, Rossi E, Törmä P, Yang B-J, 2025, "Quantum Geometry in Quantum Materials", *arXiv:250100098 [cond-mat.mes-hall]*, 1–33.
- [30] Serlin M, Tschirhart CL, Polshyn H, Zhang Y, Zhu J, Watanabe K, Taniguchi T, Balents L, Young AF, 2020, "Intrinsic quantized anomalous Hall effect in a moiré heterostructure", *Science* **367**, 900–903.
- [31] Chen G, Sharpe AL, Fox EJ, Zhang YH, Wang S, Jiang L, Lyu B, Li H, Watanabe K, Taniguchi T, Shi Z, Senthil T, Goldhaber-Gordon D, Zhang Y, Wang F, 2020, "Tunable correlated Chern insulator and ferromagnetism in a moiré superlattice", *Nature* **579**, 56–61.
- [32] Tong WY, Gong SJ, Wan X, Duan CG, 2016, "Concepts of ferrovalley material and anomalous valley Hall effect", *Nature Commun.* **7**, 13612.
- [33] Han T, Lu Z, Scuri G, Sung J, Wang J, Han T, Watanabe K, Taniguchi T, Fu L, Park H, Ju L, 2023, "Orbital multiferroicity in pentalayer rhombohedral graphene", *Nature* **623**, 41–47.
- [34] de Oteyza DG, Frederiksen T, 2022, "Carbon-based nanostructures as a versatile platform for tunable π -magnetism", *J. Phys. Condens. Matter.* **34**, 443001.
- [35] Heinrich AJ, Oliver WD, Vandersypen LMK, Ardavan A, Sessoli R, Loss D, Jayich AB, Fernandez-Rossier J, Laucht A, Morello A, 2021, "Quantum-coherent nanoscience", *Nature Nanotechnol.* **16**, 1318–1329.

- [36] The Decadal Plan for Semiconductors (2021). Semiconductor Research Corporation.
- [37] Ramesh R, Salahuddin S, Datta S, Diaz CH, Nikonov DE, Young IA, Ham D, Chang MF, Khwa WS, Lele AS, Binek C, Huang YL, Sun YC, Chu YH, Prasad B, Hoffmann M, Hu JM, Yao Z, Bellaiche L, Wu P, Cai J, Appenzeller J, Datta S, Camsari KY, Kwon J, Incorvia JAC, Asselberghs I, Ciubotaru F, Couet S, Adelman C, Zheng Y, Lindenberg AM, Evans PG, Ercius P, Radu IP, 2024, "Roadmap on low-power electronics", *Appl. Phys. Lett. Mater.* **12**, 099201.
- [38] IEEE International Roadmap for Devices and Systems, "Beyond CMOS and Emerging Materials Integration." Institute of Electrical and Electronics Engineers, 2023
- [39] Parthasarathy A, Rakheja S, 2019, "Dynamics of magnetoelectric reversal of an antiferromagnetic domain", *Phys. Rev. Appl.* **11**, 034051.
- [40] Lee Y, Kim C, Son S, Cui J, Park G, Zhang KX, Oh S, Cheong H, Kleibert A, Park JG, 2024, "Imaging Thermally Fluctuating Néel Vectors in van der Waals Antiferromagnet NiPS_3 ", *Nano Lett.* **24**, 6043–6050.
- [41] Mahmood A, Echtenkamp W, Street M, Wang JL, Cao S, Komesu T, Dowben PA, Buragohain P, Lu H, Gruverman A, Parthasarathy A, Rakheja S, Binek C, 2021, "Voltage controlled Néel vector rotation in zero magnetic field", *Nature Commun.* **12**, 1674.
- [42] Li D, Lee K, Wang BY, Osada M, Crossley S, Lee HR, Cui Y, Hikita Y, Hwang HY, 2019, "Superconductivity in an infinite-layer nickelate", *Nature* **572**, 624–627.
- [43] Sun H, Huo M, Hu X, Li J, Liu Z, Han Y, Tang L, Mao Z, Yang P, Wang B, Cheng J, Yao DX, Zhang GM, Wang M, 2023, "Signatures of superconductivity near 80 K in a nickelate under high pressure", *Nature* **621**, 493–498.
- [44] Zhu Y, Peng D, Zhang E, Pan B, Chen X, Chen L, Ren H, Liu F, Hao Y, Li N, Xing Z, Lan F, Han J, Wang J, Jia D, Wo H, Gu Y, Gu Y, Ji L, Wang W, Gou H, Shen Y, Ying T, Chen X, Yang W, Cao H, Zheng C, Zeng Q, Guo JG, Zhao J, 2024, "Superconductivity in pressurized trilayer $\text{La}_4\text{Ni}_3\text{O}_{10-\delta}$ single crystals", *Nature* **631**, 531–536.
- [45] Shi M, Peng D, Fan K, Xing Z, Yang S, Wang Y, Li H, Wu R, Du M, Ge B, Zeng Z, Zeng Q, Ying J, Wu T, Chen X 2025 "Pressure induced superconductivity in hybrid Ruddlesden–Popper $\text{La}_5\text{Ni}_3\text{O}_{11}$ single crystals", *Nature Phys.* **21**, <https://www.nature.com/articles/s41567-025-03023-3>
- [46] Ko EK, Yu Y, Liu Y, Bhatt L, Li J, Thampy V, Kuo CT, Wang BY, Lee Y, Lee K, Lee JS, Goodge BH, Muller DA, Hwang HY, 2025, "Signatures of ambient pressure superconductivity in thin film $\text{La}_3\text{Ni}_2\text{O}_7$ ", *Nature* **638**, 935–940.
- [47] Zhou G, Lv W, Wang H, Nie Z, Chen Y, Li Y, Huang H, Chen WQ, Sun YJ, Xue QK, Chen Z, 2025, "Ambient-pressure superconductivity onset above 40 K in $(\text{La,Pr})_3\text{Ni}_2\text{O}_7$ films", *Nature* **640**, 641–646.
- [48] Liu Y, Ko EK, Tarn Y, Bhatt L, Li J, Thampy V, Goodge BH, Muller DA, Raghu S, Yu Y, Hwang HY, 2025, "Superconductivity and normal-state transport in compressively strained $\text{La}_2\text{PrNi}_2\text{O}_7$ thin films", *Nature Mater.* <https://doi.org/10.1038/s41563-025-02258-y>
- [49] Wang N, Wang G, Shen X, Hou J, Luo J, Ma X, Yang H, Shi L, Dou J, Feng J, Yang J, Shi Y, Ren Z, Ma H, Yang P, Liu Z, Liu Y, Zhang H, Dong X, Wang Y, Jiang K, Hu J, Nagasaki S, Kitagawa K, Calder S, Yan J, Sun J, Wang B, Zhou R, Uwatoko Y, Cheng J, 2024, "Bulk high-temperature superconductivity in pressurized tetragonal $\text{La}_2\text{PrNi}_2\text{O}_7$ ", *Nature* **634**, 579–584.
- [50] Dong Z, Huo M, Li J, Li J, Li P, Sun H, Gu L, Lu Y, Wang M, Wang Y, Chen Z, 2024,

- "Visualization of oxygen vacancies and self-doped ligand holes in $\text{La}_3\text{Ni}_2\text{O}_{7-\delta}$ ", *Nature* **630**, 847–852.
- [51] Zhang Y-H, Vishwanath A, 2025, "Chiral Superconductivity in the Flat bands of Rhombohedral Graphene", *Journal Club J. Condens. Matter. Phys.* https://doi.org/10.36471/JCCM_February_2025_02
- [52] Schnyder AP, Brydon PMR, 2015, "Topological surface states in nodal superconductors", *J Phys Condens Matter* **27**, 243201.
- [53] Biswas PK, Ghosh SK, Zhao JZ, Mayoh DA, Zhigadlo ND, Xu X, Baines C, Hillier AD, Balakrishnan G, Lees MR, 2021, "Chiral singlet superconductivity in the weakly correlated metal LaPt_3P ", *Nature Commun* **12**, 2504.
- [54] Mackenzie AP, Scaffidi T, Hicks CW, Maeno Y, 2017, "Even odder after twenty-three years: The superconducting order parameter puzzle of Sr_2RuO_4 ", *npj Quantum Mater.* **2**, 40.
- [55] Cao Y, Fatemi V, Fang S, Watanabe K, Taniguchi T, Kaxiras E, Jarillo-Herrero P, 2018, "Unconventional superconductivity in magic-angle graphene superlattices", *Nature* **556**, 43–50.
- [56] Yankowitz M, Chen S, Polshyn H, Zhang Y, Watanabe K, Taniguchi T, Graf D, Young AF, Dean CR, 2019, "Tuning superconductivity in twisted bilayer graphene", *Science* **363**, 1059–1064.
- [57] Lu X, Stepanov P, Yang W, Xie M, Aamir MA, Das I, Urgell C, Watanabe K, Taniguchi T, Zhang G, Bachtold A, MacDonald AH, Efetov DK, 2019, "Superconductors, orbital magnets and correlated states in magic-angle bilayer graphene", *Nature* **574**, 653–657.
- [58] Chen G, Sharpe AL, Gallagher P, Rosen IT, Fox EJ, Jiang L, Lyu B, Li H, Watanabe K, Taniguchi T, Jung J, Shi Z, Goldhaber-Gordon D, Zhang Y, Wang F, 2019, "Signatures of tunable superconductivity in a trilayer graphene moiré superlattice", *Nature* **572**, 215–219.
- [59] Han T, Lu Z, Hadjri Z, Shi L, Wu Z, Xu W, Yao Y, Cotten AA, Sharifi Sedeh O, Weldeyesus H, Yang J, Seo J, Ye S, Zhou M, Liu H, Shi G, Hua Z, Watanabe K, Taniguchi T, Xiong P, Zumbühl DM, Fu L, Ju L, 2025, "Signatures of chiral superconductivity in rhombohedral graphene", *Nature*. <https://doi.org/10.1038/s41586-025-09169-7>
- [60] Das Sarma S, Freedman M, Nayak C, 2015, "Majorana zero modes and topological quantum computation", *npj Quantum Information* **1**, 15001; doi:10.1038/npjqi.2015.1
- [61] Frolov S, 2021 Quantum computing's reproducibility crisis: Majorana fermions", *Nature* **592** 350
- [62] Mann A 2025 "Corrected study rekindles debate over Microsoft's quantum computing research" *Science* 389; doi: 10.1126/science.z44ot62
- [63] Okuda Y, Nomura R 2012 "Surface Andreev bound states of superfluid ^3He and Majorana fermions", *J. Phys. Cond.: Matter* **24** 343201; doi 10.1088/0953-8984/24/34/343201
- [64] Wilczek F, 1982, "Quantum Mechanics of Fractional Spin Particles", *Phys. Rev. Lett.* **49**, 957; doi: 10.1103/PhysRevLett.49.957
- [65] Wilczek F, 1991 "Anyons for anyone", *Phys. World* **4** 40
- [66] Yazdani A, Jones BA, Lutz CP, Crommie MF, Eigler DM, 1997, "Probing the local effects of magnetic impurities on superconductivity", *Science* **275**, 1767–1770.
- [67] Heinrich BW, Pascual JI, Franke KJ, 2018, "Single magnetic adsorbates on s-wave superconductors", *Prog. Surf. Sci.* **93**, 1–19.
- [68] Soldini MO, Küster F, Wagner G, Das S, Aldarawsheh A, Thomale R, Lounis S, Parkin

- SSP, Sessi P, Neupert T, 2023, "Two-dimensional Shiba lattices as a possible platform for crystalline topological superconductivity", *Nature Phys.* **19**, 1848–1854.
- [69] Silva JPB, Alcalá R, Avci UE, Barrett N, Bégon-Lours L, Borg M, Byun S, Chang SC, Cheong SW, Choe DH, Coignus J, Deshpande V, Dimoulas A, Dubourdieu C, Fina I, Funakubo H, Grenouillet L, Gruverman A, Heo J, Hoffmann M, Hsain HA, Huang FT, Hwang CS, Iñiguez J, Jones JL, Karpov I V., Kersch A, Kwon T, Lancaster S, Lederer M, Lee Y, Lomenzo PD, Martin LW, Martin S, Migita S, Mikolajick T, Noheda B, Park MH, Rabe KM, Salahuddin S, Sánchez F, Seidel K, Shimizu T, Shiraishi T, Slesazeck S, Toriumi A, Uchida H, Vilquin B, Xu X, Ye KH, Schroeder U, 2023, "Roadmap on ferroelectric hafnia- and zirconia-based materials and devices", *APL Mater.* **11**, 0–70.
- [70] Nukala P, Ahmadi M, Wei Y, Graaf S De, Stylianidis E, Chakraborty T, Matzen S, Zandbergen HW, Björling A, Mannix D, Carbone D, Kooi B, Noheda B, 2021, "Reversible oxygen migration and phase transitions in hafnia-based ferroelectric devices", *Science* **372**, 630–635.
- [71] Lee HJ, Lee M, Lee K, Jo J, Yang H, Kim Y, Chae SC, Waghmare U, Lee JH, 2020, "Scale-free ferroelectricity induced by flat phonon bands in HfO_2 ", *Science* **369**, 1343–1347.
- [72] Kittel C, 1951, "Theory of antiferroelectric crystals", *Phys Rev* **82**, 729–732.
- [73] Blinov LM, Fridkin VM, Palto SP, Bune AV, Dowben PA, Ducharme S, 2000 "Two-Dimensional Ferroelectrics", *Physics Uspekhi* **43** 243–257; doi: 10.1070/PU2000v043n03ABEH000639
- [74] Tang Z, Hu Y, Rogée L, Liu D, Lau SP 2025, "Towards Multiferroicity in Two-Dimensional Van Der Waals Materials: Challenges and Opportunities", *Chemistry of Materials* **37**, 4925–4934; doi: 10.1021/acs.chemmater.5c01047
- [75] Lavrentovich OD 2020, "Ferroelectric nematic liquid crystal, a century in waiting", *Proc. Natl. Acad. Sci.* **117** 14629–14631; doi: 10.1073/pnas.2008947117
- [76] Chen X, Korblova E, Dong D, Clark NA 2020 "First-principles experimental demonstration of ferroelectricity in a thermotropic nematic liquid crystal: Polar domains and striking electro-optics. *Proc. Natl. Acad. Sci. U.S.A.* **117**, 14021–14031; doi: 10.1073/pnas.2002290117
- [77] Kumari P, Basnet B, Lavrentovich MO, Lavrentovich OD 2024 "Chiral ground states of ferroelectric liquid crystals", *Science* **383**, 1364–1368; doi: 10.1126/science.adl0834
- [78] Zhang L, Pang B, Chen YB, Chen Y, 2018, "Review of Spin–Orbit Coupled Semimetal SrIrO_3 in Thin Film Form", *Crit. Rev. Solid State Mater. Sci.* **43**, 367–391.
- [79] Schütz P, Di Sante D, Dudy L, Gabel J, Stübinger M, Kamp M, Huang Y, Capone M, Husanu MA, Strocov VN, Sangiovanni G, Sing M, Claessen R, 2017, "Dimensionality-Driven Metal-Insulator Transition in Spin-Orbit-Coupled SrIrO_3 ", *Phys. Rev. Lett.* **119**, 256404.
- [80] Zhang L, Jiang X, Xu X, Hong X, 2020, "Abrupt enhancement of spin-orbit scattering time in ultrathin semimetallic SrIrO_3 close to the metal-insulator transition", *APL Mater.* **8**, 051108.
- [81] Empante TA, Martinez A, Wurch M, Zhu Y, Geremew AK, Yamaguchi K, Isarraraz M, Rumyantsev S, Reed EJ, Balandin AA, Bartels L, 2019, "Low Resistivity and High Breakdown Current Density of 10 nm Diameter van der Waals TaSe_3 Nanowires by Chemical Vapor Deposition", *Nano Lett.* **19**, 4355–4361.
- [82] Geremew A, Bloodgood MA, Aytan E, Woo BWK, Corber SR, Liu G, Bozhilov K,

- Salguero TT, Rumyantsev S, Rao MP, Balandin AA, 2018, "Current Carrying Capacity of Quasi-1D ZrTe₃ Van der Waals Nanoribbons", *IEEE Electron Device Lett.* **39**, 735–738.
- [83] Hoesch M, Gannon L, Shimada K, Parrett BJ, Watson MD, Kim TK, Zhu X, Petrovic C, 2019, "Disorder Quenching of the Charge Density Wave in ZrTe₃", *Phys. Rev. Lett.* **122**, 017601.
- [84] Yue L, Xue S, Li J, Hu W, Barbour A, Zheng F, Wang L, Feng J, Wilkins SB, Mazzoli C, Comin R, Li Y, 2020, "Distinction between pristine and disorder-perturbed charge density waves in ZrTe₃", *Nature Commun.* **11**, 98.
- [85] Zhu X, Ning W, Li L, Ling L, Zhang R, Zhang J, Wang K, Liu Y, Pi L, Ma Y, Du H, Tian M, Sun Y, Petrovic C, Zhang Y, 2016, "Superconductivity and Charge Density Wave in ZrTe_{3-x}Se_x", *Sci. Rept.* **6**, 26974.
- [86] Takahashi S, Sambongi T, Okada S, 1983, "Conduction Properties of ZrTe₃", *J. Phys* **44**, C3-1733-C3-1736.
- [87] Tsuchiya S, Matsubayashi K, Yamaya K, Takayanagi S, Tanda S, Uwatoko Y, 2017, "Effects of pressure and magnetic field on superconductivity in ZrTe₃: Local pair-induced superconductivity", *New J. Phys.* **19**, 063004.
- [88] Eaglesham DJ, Steeds JW, Wilson JA, 1984, "Electron microscope study of superlattices in ZrTe₃", *J. Phys. C: Solid State Phys.* **17**, L697–L698.
- [89] Lauk N, Sinclair N, Barzanjeh S, Covey JP, Saffman M, Spiropulu M, Simon C, 2020, "Perspectives on quantum transduction", *Quantum Sci. Technol.* **5**, 020501.
- [90] Lambert NJ, Rueda A, Sedlmeir F, Schwefel HGL, 2020, "Coherent Conversion Between Microwave and Optical Photons—An Overview of Physical Implementations", *Adv. Quantum Technol.* **3**, 1900077.
- [91] Lemonde MA, Meesala S, Sipahigil A, Schuetz MJA, Lukin MD, Loncar M, Rabl P, 2018, "Phonon Networks with Silicon-Vacancy Centers in Diamond Waveguides", *Phys. Rev. Lett.* **120**, 213603.
- [92] Chen HY, MacQuarrie ER, Fuchs GD, 2018, "Orbital State Manipulation of a Diamond Nitrogen-Vacancy Center Using a Mechanical Resonator", *Phys. Rev. Lett.* **120**, 167401.
- [93] Chen H, Opondo NF, Jiang B, Macquarrie ER, Daveau RS, Bhawe SA, Fuchs GD, 2019, "Engineering Electron-Phonon Coupling of Quantum Defects to a Semiconfocal Acoustic Resonator", *Nano Lett.* **19**, 7021–7027.
- [94] Hucul D, Inlek I V., Vittorini G, Crocker C, Debnath S, Clark SM, Monroe C, 2015, "Modular entanglement of atomic qubits using photons and phonons", *Nature Phys.* **11**, 37–42.
- [95] Vermersch B, Guimond PO, Pichler H, Zoller P, 2017, "Quantum State Transfer via Noisy Photonic and Phononic Waveguides", *Phys. Rev. Lett.* **118**, 1–6.
- [96] Safavi-Naeini AH, Van Thourhout D, Baets R, Van Laer R, 2019, "Controlling phonons and photons at the wavelength scale: integrated photonics meets integrated phononics", *Optica* **6**, 213.
- [97] Fransson J, Bird JP, 2025, "Coherent phonon source based on electron spin resonance in a quantum-dot qubit", *Sci. Rept.* **15**, 13616.
- [98] Qiu Z, Vaklinova K, Huang P, Grzeszczyk M, Watanabe K, Taniguchi T, Novoselov KS, Lu J, Koperski M, 2024, "Atomic and Electronic Structure of Defects in hBN: Enhancing Single-Defect Functionalities", *ACS Nano* **18**, 24035–24043.
- [99] Zhang L, Niu Q, 2015, "Chiral Phonons at High-Symmetry Points in Monolayer Hexagonal Lattices", *Phys. Rev. Lett.* **115**, 115502.

- [100] Zhu H, Yi J, Li MY, Xiao J, Zhang L, Yang CW, Kaindl RA, Li LJ, Wang Y, Zhang X, 2018, "Observation of chiral phonons", *Science* **359**, 579–582.
- [101] Fransson J, 2023, "Chiral phonon induced spin polarization", *Phys. Rev. Res.* **5**, L022039.
- [102] Hamada M, Minamitani E, Hirayama M, Murakami S, 2018, "Phonon Angular Momentum Induced by the Temperature Gradient", *Phys. Rev. Lett.* **121**, 175301.
- [103] D'Alessio L, Polkovnikov A, 2013, "Many-body energy localization transition in periodically driven systems", *Ann. Phys. (N Y)* **333**, 19–33.
- [104] Bukov M, D'Alessio L, Polkovnikov A, 2015, "Universal high-frequency behavior of periodically driven systems: From dynamical stabilization to Floquet engineering", *Adv. Phys.* **64**, 139–226.
- [105] Oka T, Kitamura S, 2019, "Floquet engineering of quantum materials", *Ann. Rev. Condens. Matter Phys.* **10**, 387–408.
- [106] Blanes S, Casas F, Oteo JA, Ros J, 2009, "The Magnus expansion and some of its applications", *Phys. Rept.* **470**, 151–238.
- [107] Eckardt A, 2017, "Colloquium: Atomic quantum gases in periodically driven optical lattices", *Rev. Mod. Phys.* **89**, 011004.
- [108] Sen A, Sen D, Sengupta K, 2021, "Analytic approaches to periodically driven closed quantum systems: Methods and applications", *J. Phys. Condens. Matter* **33**, 443003.
- [109] Banerjee T, Sengupta K, 2025, "Emergent symmetries in prethermal phases of periodically driven quantum systems", *J. Phys. Condens. Matter* **37**, 133002.
- [110] D'Alessio L, Kafri Y, Polkovnikov A, Rigol M, 2016, "From quantum chaos and eigenstate thermalization to statistical mechanics and thermodynamics", *Adv. Phys.* **65**, 239–362.
- [111] Bloch I, Dalibard J, Zwerger W, 2008, "Many-body physics with ultracold gases", *Rev. Mod. Phys.* **80**, 885–964.
- [112] Han JE, Aron C, Chen X, Mansaray I, Han JH, Kim KS, Randle M, Bird JP, 2023, "Correlated insulator collapse due to quantum avalanche via in-gap ladder states", *Nature Commun.* **14**, 2936.
- [113] Sieberer LM, Buchhold M, Marino J, Diehl S, 2025, "Universality in driven open quantum matter", *Rev. Mod. Phys.* **97**, 025004.
- [114] Mori T, 2023, "Floquet States in Open Quantum Systems", *Ann. Rev. Condens. Matter Phys.* **14**, 35–56.
- [115] Dziarmaga J, 2010, "Dynamics of a quantum phase transition and relaxation to a steady state", *Adv. Phys.* **59**, 1063–1189.
- [116] Polkovnikov A, Sengupta K, Silva A, Vengalattore M, 2011, "Colloquium: Nonequilibrium dynamics of closed interacting quantum systems", *Rev. Mod. Phys.* **83**, 863–883.
- [117] Dutta A, Aeppli G, Chakrabarti BK, Divakaran U, Rosenbaum TF, Sen D, Quantum phase transitions in transverse field spin models: from statistical physics to quantum information. Cambridge University Press, Cambridge, 2015
- [118] Chandra AK, Das A, Chakrabarti BK (eds), Lecture Notes in Physics 802: Quantum Quenching, Annealing and Computation. Springer, Berlin, Heidelberg, 2010
- [119] Shevchenko SN, Ashhab S, Nori F, 2010, "Landau-Zener-Stückelberg interferometry", *Phys. Rept.* **492**, 1–30.
- [120] Kibble T, Srivastava A, 2013, "Condensed matter analogues of cosmology. Preface.", *J. Phys. Condens. Matter* **25**, 400301.

- [121] Hong X, Kim J, Shi SF, Zhang Y, Jin C, Sun Y, Tongay S, Wu J, Zhang Y, Wang F, 2014, "Ultrafast charge transfer in atomically thin MoS₂/WS₂ heterostructures", *Nature Nanotechnol.* **9**, 682–686.
- [122] Guo Z, Wan Y, Yang M, Snaider J, Zhu K, Huang L, 2017, "Long-range hot-carrier transport in hybrid perovskites visualized by ultrafast microscopy", *Science* **356**, 59–62.
- [123] Sobota JA, He Y, Shen ZX, 2021, "Angle-resolved photoemission studies of quantum materials", *Rev. Mod. Phys.* **93**, 025006.
- [124] Boschini F, Zonno M, Damascelli, A. 2024 Time-resolved ARPES studies of quantum materials. *Rev. Mod. Phys.* **96**, 015003.
- [125] Na M, Mills A K, Jones D J, 2023, Advancing time- and angle-resolved photoemission spectroscopy: the role of ultrafast laser development. *Phys. Rep.* **1036**, 1–47; doi: [10.1016/j.physrep.2023.09.005](https://doi.org/10.1016/j.physrep.2023.09.005)
- [126] Guo C, Meng X, Fu H, Wang Q, Wang H, Tian Y, Peng J, Ma R, Weng Y, Meng S, Wang E, Jiang Y, 2020, "Probing Nonequilibrium Dynamics of Photoexcited Polarons on a Metal-Oxide Surface with Atomic Precision", *Phys. Rev. Lett.* **124**, 206801.
- [127] Filippetto D, Musumeci P, Li RK, Siwick BJ, Otto MR, Centurion M, Nunes JPF, 2022, "Ultrafast electron diffraction: Visualizing dynamic states of matter", *Rev. Mod. Phys.* **94**, 045004.
- [128] Cocker TL, Peller D, Yu P, Repp J, Huber R, 2016, "Tracking the ultrafast motion of a single molecule by femtosecond orbital imaging", *Nature* **539**, 263–267.
- [129] Schuler B, Cochrane KA, Kastl C, Barnard ES, Wong E, Borys NJ, Schwartzberg AM, Ogletree DF, De Abajo FJG, Weber-Bargioni A, 2020, "Electrically driven photon emission from individual atomic defects in monolayer WS₂", *Sci. Adv.* **6**, eabb5988.
- [130] Yu C, Jiang S, Lu R, 2019, "High order harmonic generation in solids: A review on recent numerical methods", *Adv. Phys. X* **4**, 1562982.
- [131] Meng S, Kaxiras E, 2008, "Real-time, local basis-set implementation of time-dependent density functional theory for excited state dynamics simulations", *J. Chem. Phys.* **129**, 054110.
- [132] Lian C, Guan M, Hu S, Zhang J, Meng S, 2018, "Photoexcitation in Solids: First-Principles Quantum Simulations by Real-Time TDDFT", *Adv. Theory Simulations* **1**, 1800055.
- [133] Jia W, Cao Z, Wang L, Fu J, Chi X, Gao W, Wang LW, 2013, "The analysis of a plane wave pseudopotential density functional theory code on a GPU machine", *Comput. Phys. Commun.* **184**, 9–18.
- [134] Jia W, Fu J, Cao Z, Wang L, Chi X, Gao W, Wang LW, 2013, "Fast plane wave density functional theory molecular dynamics calculations on multi-GPU machines", *J. Comput. Phys.* **251**, 102–115.
- [135] Tancogne-Dejean N, Oliveira MJT, Andrade X, Appel H, Borca CH, Le Breton G, Buchholz F, Castro A, Corni S, Correa AA, De Giovannini U, Delgado A, Eich FG, Flick J, Gil G, Gomez A, Helbig N, Hübener H, Jestädt R, Jornet-Somoza J, Larsen AH, Lebedeva I V., Lüders M, Marques MAL, Ohlmann ST, Pipolo S, Rampp M, Rozzi CA, Strubbe DA, Sato SA, Schäfer C, Theophilou I, Welden A, Rubio A, 2020, "Octopus, a computational framework for exploring light-driven phenomena and quantum dynamics in extended and finite systems", *J. Chem. Phys.* **152**, 124119.
- [136] Attaccalite C, Grüning M, Marini A, 2011, "Real-time approach to the optical properties of solids and nanostructures: Time-dependent Bethe-Salpeter equation", *Phys. Rev. B* **84**,

- 245110.
- [137] Chan YH, Qiu DY, da Jornada FH, Louie SG, 2021, "Giant exciton-enhanced shift currents and direct current conduction with subbandgap photo excitations produced by many-electron interactions", *Proc. Natl. Acad. Sci.* **118**, e1906938118.
- [137] Shi J, Turkowski V, Rahman TS, 2023, "Dark-exciton energy splitting in monolayer WSe₂: Insights from time-dependent density functional theory", *Phys. Rev. B* **107**, 155431.
- [138] Yu Y, Turkowski V, Hachtel JA, Puzdsky AA, Ievlev A V., Din NU, Harris SB, Iyer V, Rouleau CM, Rahman TS, Geohegan DB, Xiao K, 2024, "Anomalous isotope effect on the optical bandgap in a monolayer transition metal dichalcogenide semiconductor", *Sci. Adv.* **10**, eadj0758.
- [139] Zhou JJ, Park J, Lu I Te, Maliyov I, Tong X, Bernardi M, 2021, "PERTURBO: A software package for ab initio electron-phonon interactions, charge transport and ultrafast dynamics", *Comput. Phys. Commun.* **264**, 107970.
- [140] Acharya SR, Turkowski V, Zhang G-p, Rahman TS, 2020 "Ultrafast electron correlations and memory effects at work: femtosecond demagnetization in Ni," *Phys. Rev. Lett.* **125**, 017202
- [141] Turkowski V, Rahman TS, 2017 "Nonadiabatic exchange-correlation kernel for strongly correlated materials," *Journal of Physics: Condensed Matter* **29**, 455601 (2017).
- [143] Akimov A V., Prezhdo O V., 2013, "The PYXAID program for non-adiabatic molecular dynamics in condensed matter systems", *J. Chem. Theory Comput.* **9**, 4959–4972.
- [144] Zheng Z, Zheng Q, Zhao J, 2022, "Spin-orbit coupling induced demagnetization in Ni: Ab initio nonadiabatic molecular dynamics perspective", *Phys. Rev. B* **105**, 085142.
- [145] Jiang X, Zheng Q, Lan Z, Saidi WA, Ren X, Zhao J, 2021, "Real-time GW-BSE investigations on spin-valley exciton dynamics in monolayer transition metal dichalcogenide", *Sci. Adv.* **7**, eabf3759.
- [146] Zheng Z, Shi Y, Zhou J-J, Prezhdo O V., Zheng Q, Zhao J, 2023, "Ab initio real-time quantum dynamics of charge carriers in momentum space", *Nature Comput. Sci.* **3**, 532–541.
- [147] Zheng Q, Chu W, Zhao C, Zhang L, Guo H, Wang Y, Jiang X, Zhao J, 2019, "Ab initio nonadiabatic molecular dynamics investigations on the excited carriers in condensed matter systems", *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **9**, e1411.
- [148] Schleder GR, Padilha ACM, Acosta CM, Costa M, Fazzio A, 2019, "From DFT to machine learning: Recent approaches to materials science - A review", *J. Phys.: Mater.* **2**, 032001.
- [149] Carrasquilla J, Melko RG, 2017, "Machine learning phases of matter", *Nature Phys.* **13**, 431–434.
- [150] Kong S, Ricci F, Guevarra D, Neaton JB, Gomes CP, Gregoire JM, 2022, "Density of states prediction for materials discovery via contrastive learning from probabilistic embeddings", *Nature Commun.* **13**, 949.
- [151] Gong X, Li H, Zou N, Xu R, Duan W, Xu Y, 2023, "General framework for E(3)-equivariant neural network representation of density functional theory Hamiltonian", *Nature Commun.* **14**, 2848.
- [152] Wang J, Wang Y, Zhang H, Yang Z, Liang Z, Shi J, Wang HT, Xing D, Sun J, 2024, "E(n)-Equivariant cartesian tensor message passing interatomic potential", *Nature Commun.* **15**, 7607.

- [153] Omranpour A, Elsner J, Lausch KN, Behler J, 2025, "Machine Learning Potentials for Heterogeneous Catalysis", *ACS Catal.* **15**, 1616–1634.
- [154] Cirac JJ, Pérez-García D, Schuch N, Verstraete F, 2021, "Matrix product states and projected entangled pair states: Concepts, symmetries, theorems", *Rev. Mod. Phys.* **93**, 045003.
- [155] Gross L, Wang ZL, Ugarte D, Mohn F, Moll N, Heer W a, Vincent P, Liljeroth P, Journet C, Meyer G, Binh VT, Poot M, Zant HSJ Van Der, Aguasca A, Bachtold A, Kim K, Zettl A, Hung P, Postma HWC, Bockrath M, Blase X, Roche S, 2009, "The Chemical Structure of a Molecule Resolved by Atomic Force Microscopy", *Science* **325**, 1110–4.
- [156] Pavlicek N, Gross L, 2017, "Generation, manipulation and characterization of molecules by atomic force microscopy", *Nat. Rev. Chem.* **1**, 0005.
- [157] Mishra S, Catarina G, Wu F, Ortiz R, Jacob D, Eimre K, Ma J, Pignedoli CA, Feng X, Ruffieux P, Fernández-Rossier J, Fasel R, 2021, "Observation of fractional edge excitations in nanographene spin chains", *Nature* **598**, 287–292.
- [158] Sellies L, Spachtholz R, Bleher S, Eckrich J, Scheuerer P, Repp J, 2023, "Single-molecule electron spin resonance by means of atomic force microscopy", *Nature* **624**, 64–68.
- [159] Piquero-Zulaica I, Lobo-Checa J, El-Fattah ZMA, Ortega JE, Klappenberger F, Auwärter W, Barth J V., 2022, "Engineering quantum states and electronic landscapes through surface molecular nanoarchitectures", *Rev. Mod. Phys.* **94**, 045008.
- [160] Rojas G, Simpson S, Chen X, Kunkel DA, Nitz J, Xiao J, Dowben PA, Zurek E, Enders A, 2012, "Surface state engineering of molecule-molecule interactions", *Phys. Chem. Chem. Phys.* **14**, 4971–4976.
- [161] Simpson S, Kunkel DA, Hooper J, Nitz J, Dowben PA, Routaboul L, Braunstein P, Doudin B, Enders A, Zurek E, 2013, "Coverage-dependent interactions at the organics-metal interface: Quinonoid zwitterions on Au(111)", *J. Phys. Chem. C* **117**, 16406–16415.
- [162] Yin R, Zhu X, Fu Q, Hu T, Wan L, Wu Y, Liang Y, Wang Z, Qiu ZL, Tan YZ, Ma C, Tan S, Hu W, Li B, Wang ZF, Yang J, Wang B, 2024, "Artificial kagome lattices of Shockley surface states patterned by halogen hydrogen-bonded organic frameworks", *Nature Commun.* **15**, 2969.
- [163] Luo H, Yu P, Li G, Yan K, 2022, "Topological quantum materials for energy conversion and storage", *Nat. Rev. Phys.* **4**, 611–624.
- [164] Wang X, Yang Q, Singh S, Borrmann H, Hasse V, Yi C, Li Y, Schmidt M, Li X, Fecher GH, Zhou D, Yan B, Felser C, 2025, "Topological semimetals with intrinsic chirality as spin-controlling electrocatalysts for the oxygen evolution reaction", *Nature Energy* **10**, 101–109.
- [165] Lew-Yee J F H, del Campo J M, Piris M 2025 "Advancing Natural Orbital Functional Calculations through Deep Learning-Inspired Techniques for Large-Scale Strongly Correlated Electron Systems" *Phys. Rev. Lett.* 134, 206401: DOI: 10.1103/PhysRevLett.134.206401
- [166] Ekanayaka TK, Hao G, Mosey A, Dale AS, Jiang X, Yost AJ, Sapkota KR, Wang GT, Zhang J, N'Diaye AT, Marshall A, Cheng R, Naeemi A, Xu X, Dowben PA, 2021, "Nonvolatile voltage controlled molecular spin-state switching for memory applications", *Magnetochemistry* **7**, 37.
- [167] (RETRACTED) Schön JH, Kloc C, 2001, "Fast organic electronic circuits based on ambipolar pentacene field-effect transistors", *Appl. Phys. Lett.* **79**, 4043–4044.
- [168] (RETRACTED) Schön JH, Kloc C, Batlogg B, 2001, " Ambipolar organic devices for

complementary logic", *Synth. Met.* **122**, 195–197.
[169] Stein E, Nahor O, Stolov M, Freger V, Petruta IM, McCulloch I, Frey GL, 2022,
"Ambipolar blend-based organic electrochemical transistors and inverters", *Nature*
Commun. **13**, 5548.