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The 2021 quantum materials roadmap

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ROADMAP

The 2021 quantum materials roadmap

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Abstract

In recent years, the notion of ‘Quantum Materials’ has emerged as a powerful unifying concept across diverse fields of science and engineering, from condensed-matter and coldatom physics to materials science and quantum computing. Beyond traditional quantum materials such as unconventional superconductors, heavy fermions, and multiferroics, the field has significantly expanded to encompass topological quantum matter, two-dimensional materials and their van der Waals heterostructures, Moiré materials, Floquet time crystals, as well as materials and devices for quantum computation with Majorana fermions. In this Roadmap collection we aim to capture a snapshot of the most recent developments in the field, and to identify outstanding challenges and emerging opportunities. The format of the Roadmap, whereby experts in each discipline share their viewpoint and articulate their vision for quantum materials, reflects the dynamic and multifaceted nature of this research area, and is meant to encourage exchanges and discussions

across traditional disciplinary boundaries. It is our hope that this collective vision will contribute to sparking new fascinating questions and activities at the intersection of materials science, condensed matter physics, device engineering, and quantum information, and to shaping a clearer landscape of quantum materials science as a new frontier of interdisciplinary scientific inquiry. We stress that this article is not meant to be a fully comprehensive review but rather an up-to-date snapshot of different areas of research on quantum materials with a minimal number of references focusing on the latest developments.

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1. Introduction

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In recent years, the notion of ‘Quantum Materials’ has emerged as a powerful unifying concept across diverse fields of science and engineering, from condensed-matter and cold-atom physics to materials science and quantum computing. Originally introduced to emphasize the exotic properties of unconventional superconductors, heavy-fermion systems, and multifunctional oxides, the definition of quantum materials has morphed into a much broader container that also encompasses research on topological properties, two-dimensional (2D) materials, and driven quantum systems. This convergence of diverse research areas is perhaps best exemplified by the coexistence of strong correlation, quantum criticality, and superconductivity in Moiré materials such as twisted bilayer graphene (TBG) [1]. With this example in mind, it is natural to broadly define quantum materials as all those versatile materials platforms that allow us to explore emergent quantum phenomena as well as their potential uses in future technology.

Apart from unconventional superconductivity and Kondo physics, one of the earliest realizations of emergent phenomena in novel materials platforms can be traced back to the discovery of graphene. This discovery has opened a new dimension to explore unconventional transport properties of massless Dirac fermions, originally predicted to only occur at unreachable high energy scales [2].

The subsequent search for Dirac physics in materials beyond graphene has brought into focus the role of intrinsic spin–orbit coupling (SOC) effects and led to the ground-breaking prediction of the existence of topological insulators (TIs) and superconductors [3–5], as well as the ensuing experimental discovery of the former class [6, 7]. Such a new class of quantum materials is characterized by topologically protected massless Dirac surface states at the edges of 2D materials (2DMs) or at the surfaces of their three-dimensional (3D) counterparts. These efforts were instrumental to the theoretical prediction and subsequent experimental discovery of Weyl fermions chalcogenide semimetals with their unique Fermi surface arcs [8, 9]. These and many other advances have clearly shown that symmetry-based topological concepts are ubiquitous in materials physics and offer unique opportunities to connect seemingly unrelated materials families and enable new discoveries.

In addition to its central role in topological quantum materials, SOC underpins a much wider array of phenomena in condensed matter. For example, in non-magnetic crystals with broken inversion symmetry, the Kramers degeneracy of electronic energy bands is lifted by SOC. This splitting arises from the interaction between the electron’s spin and the Rashba field, that is the effective magnetic field that electrons experience in their rest frame when moving in an electric field. The Rashba field generates a wide variety of fascinating quantum phenomena, including the spin Hall effect (SHE), the spin–orbit torque (SOT), chiral magnons, electric-dipole spin resonance, skyrmions [10], and also Majorana fermions [11].

Moving beyond bulk 3D and 2DMs, tremendous advances in fabrication techniques have enabled the development of ultraclean van der Waals (vdW) heterostructures based on atomically-thin 2D crystals. In this new class of artificial materials, unique proximity effects that are absent in conventional materials lead to novel physical phenomena. Ground-breaking examples include topological order driving the quantum SHE in tungsten ditelluride [12], spin-charge conversion in graphene in proximity with transition-metal dichalcogenides [13], the demonstration of room temperature 2D ferromagnetism [14], the quantum anomalous effect [15, 16], the observation of charge density waves (CDWs) and light-driven Floquet states [17], and the discovery of superconductivity in TBG [18, 19]. In addition, recent work on materials with strong SOC reported evidences of the long-sought after Majorana fermions. The Majorana particle is unique in high-energy physics insofar as it is its own antiparticle [20, 21]. Initial evidence for these particles has been obtained from the exploration of phenomena emerging at the boundary between strong SOC materials and superconductors, for example ballistic InSb nanowire devices and epitaxial Al–InAs nanowires [22]. Recent work also reported evidence of Majoranas in an iron selenium telluride superconductor [23]. Understanding these emerging quasiparticles is not only of fundamental interest, but it might also lead to applications, for example as the building blocks of non-Abelian topological quantum computers [24].

The merging of strong correlations with topological matter creates yet another dimension for quantum materials, which might help in understanding and controlling complex phenomena such as high critical temperature superconductivity, the Kondo effect, and quantum criticality. Taking a broader perspective, it is

particularly remarkable that the nascent family of new quantum materials has ignited and accelerated efforts towards the development of next generation quantum technologies (QTs). QT explicitly address individual quantum states and make use of the ‘strangeness’ of quantum physics such as superposition and entanglement, with the goal to build practical solutions for quantum computation, quantum sensing, and quantum metrology [25]. While quantum computers may still be some way in the future, quantum materials are already here to respond to the challenges posed by quantum computation, and to offer unique opportunities to imagine and realize the device architectures and computation paradigms that will be needed to achieve the so-called ‘quantum supremacy’.

As the library of quantum materials grows larger, it is becoming increasingly important to be able to leverage modern data science techniques to catalogue, search, and design new quantum materials [26, 27]. Machine learning (ML) and related artificial intelligence algorithms are expected to play a central role in this area. ML techniques can assist the high-throughput search for suitable materials for given applications, by harvesting the massive amount of raw data generated and stored by the computational materials science community. ML is particularly useful to identify patterns within large amounts of complex data, and many groups started to explore these methodologies for extracting knowledge and insight from materials databases [28]. ML is also seen as a powerful tool to advance the identification of quantum phase transitions and to deepen our understanding of many-body physics and quantum topological matter [25]. This nascent field holds great promise and is expected to play a fundamental role in progressing towards new materials solutions for next-generation QTs.

In this vast and fast-moving research area, the aim of this Roadmap is to capture a snapshot of the latest developments in the field, and to offer a broad perspective on emerging horizons in quantum materials research. Although the field is already too big to be covered in all its aspects, we believe that many of the cornerstone materials driving innovation and underpinning emerging quantum phenomena are addressed in this collection.

It is often the case that radically new ideas emerge from scientific controversies and puzzling experimental data that challenge existing paradigms. It is our hope that, by pointing out such directions where further work and more in-depth analysis are called for, this roadmap will be able to stimulate new explorations and contribute to shaping this promising research field.

By giving voice to leading groups working on quantum materials from very different perspectives, we further expect that new fascinating questions will emerge at the intersection of materials science, condensed matter physics, device engineering, and quantum information, making quantum materials research a new frontier of scientific inquiry across disciplinary boundaries. We hope that our review will contribute to inspire much future work in the field.

Acknowledgments

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2. Complex oxides

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Status

After decades of work on bulk systems that led to the discovery of colossal magnetoresistance, multiferroicity and high- T_C superconductivity, the field of complex oxides is now largely focused on thin film heterostructures. In such systems, materials with different properties can be assembled leading to cross-coupling between functionalities and giant responses. Often, interfaces between dissimilar materials exhibit unexpected physics arising from inversion-symmetry breaking and charge/spin/orbital reconstruction. Among a cornucopia of materials and physical effects explored in the last decade, three main families of quantum oxide systems have attracted a lot of attention: multiferroics, 2D electron gases (2DEGs) and rare-earth nickelates $RNiO_3$ (R: rare-earth).

Multiferroics simultaneously possess at least two ferroic orders and are usually antiferromagnetic and ferroelectric. Aside from having brought several new physical concepts such as improper ferroelectricity (induced by non-collinear spin order breaking inversion symmetry) or electromagnons (coupled lattice and spin excitations), multiferroics are attractive because the magnetoelectric coupling between spin and dipole orders allows for an electric field control of magnetism. Magnetoelectric coupling has fuelled an intense research activity in single-phase materials such as $BiFeO_3$ [29] as well as in bilayers (combining a ferroelectric and a ferromagnet for instance) and in composites, with a view towards magnetoelectric sensors, memories or transistors. $BiFeO_3$, as well as some other ferroelectrics and multiferroics, also displays conductive domain walls between adjacent ferroelectric domains, which can be functionalized into nanoscale devices with rewritable circuitry.

Research on oxide 2DEGs was born with the discovery of a high-mobility metallic state at the interface between two insulators, $LaAlO_3$ and $SrTiO_3$ (STO) [30]. The 2DEG was later found to be superconducting and to possess a sizeable Rashba-type SOC [31], both highly tunable by a gate voltage. A similar 2DEG can also form at the surface of STO [32] and by depositing a thin layer of a reactive metal such as Al on STO. Parallel to this research, huge progress was also made in oxide thin film synthesis, leading for instance to the observation of the integer and fractional quantum Hall effects in ultrapure $ZnO/(Mg,Zn)O$ quantum wells (QWs) [33] (figure 1(b)).

Another important direction in complex oxides has been the investigation of perovskite nickelate thin film heterostructures. Except for $LaNiO_3$, these compounds exhibit a metal–insulator transition at a temperature increasing with rare-earth atomic number. They also harbour a complex antiferromagnetic order at low temperature. Predictions of cuprate-like conductivity in carefully engineered nickelate superlattices [34] stimulated an intense research effort and superconductivity was finally found in nickelates in 2019, albeit through a different, chemistry-based approach to achieve an infinite-layer compound with similarities to cuprates [35] (figure 1(c)).

Current and future challenges

Although complex oxides display a vast array of functionalities, most are restricted to low temperatures or their performance remains insufficient for room-temperature operation. Thus, an important challenge for the field is to design and realize materials with superior properties, eventually leading to applications. The field of multiferroics is particularly illustrative since $BiFeO_3$ has been and remains the only practical room-temperature multiferroic. Yet, its relatively weak magnetoelectric coupling complicates its integration into advanced devices such as the magnetoelectric spin–orbit (MESO) transistor proposed by Intel [37] (see figure 2(a)), even though major progress was realized in the recent years [29]. The second leg of the MESO transistor is a spin–orbit element and the very efficient properties of spin–charge interconversion displayed by STO 2DEGs makes them interesting candidates for this application [31]. Yet, the room-temperature response still falls short by about one order of magnitude.

In terms of fundamental science, the emergence of chiral and topological spin and dipole textures [36] in magnetic oxides, ferroelectrics and multiferroics is opening an exciting new direction, with a view towards the electrical control of the generation and motion of such objects. Beyond STO 2DEGs, new systems with high mobilities have emerged such as stannates (e.g. La-doped $BaSnO_3$) or $SrVO_3$. SOC has also been introduced as a key ingredient, adding to the usual spin, charge, lattice and orbital degrees of freedom, leading to exotic phases of matter, as in perovskite iridates. New superconducting phases have been discovered in ruthenates and more recently in nickelates [35], and much of their physics is still elusive. Despite various predictions and experimental attempts, oxide-based TIs have not yet been discovered.

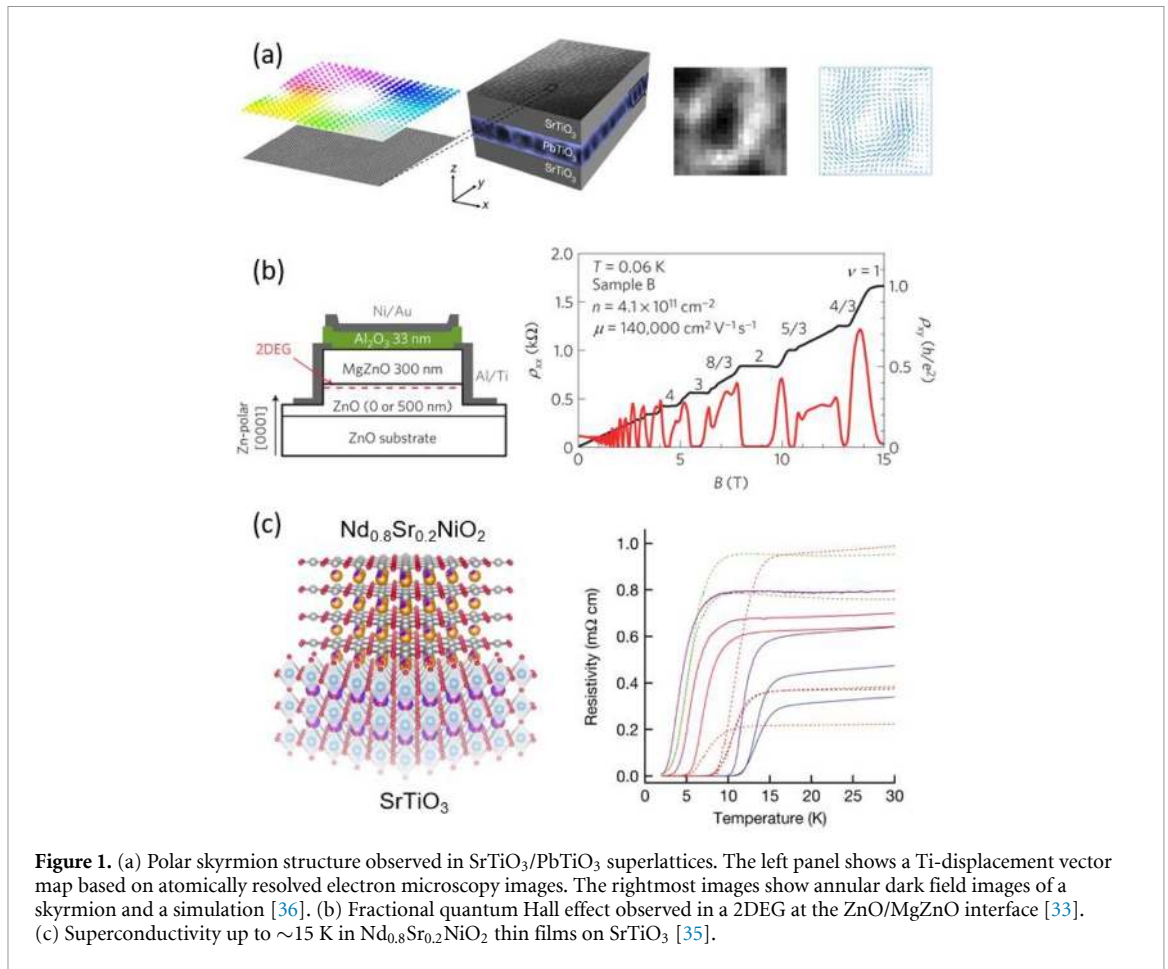


Figure 1. (a) Polar skyrmion structure observed in SrTiO₃/PbTiO₃ superlattices. The left panel shows a Ti-displacement vector map based on atomically resolved electron microscopy images. The rightmost images show annular dark field images of a skyrmion and a simulation [36]. (b) Fractional quantum Hall effect observed in a 2DEG at the ZnO/MgZnO interface [33]. (c) Superconductivity up to ~15 K in Nd_{0.8}Sr_{0.2}NiO₂ thin films on SrTiO₃ [35].

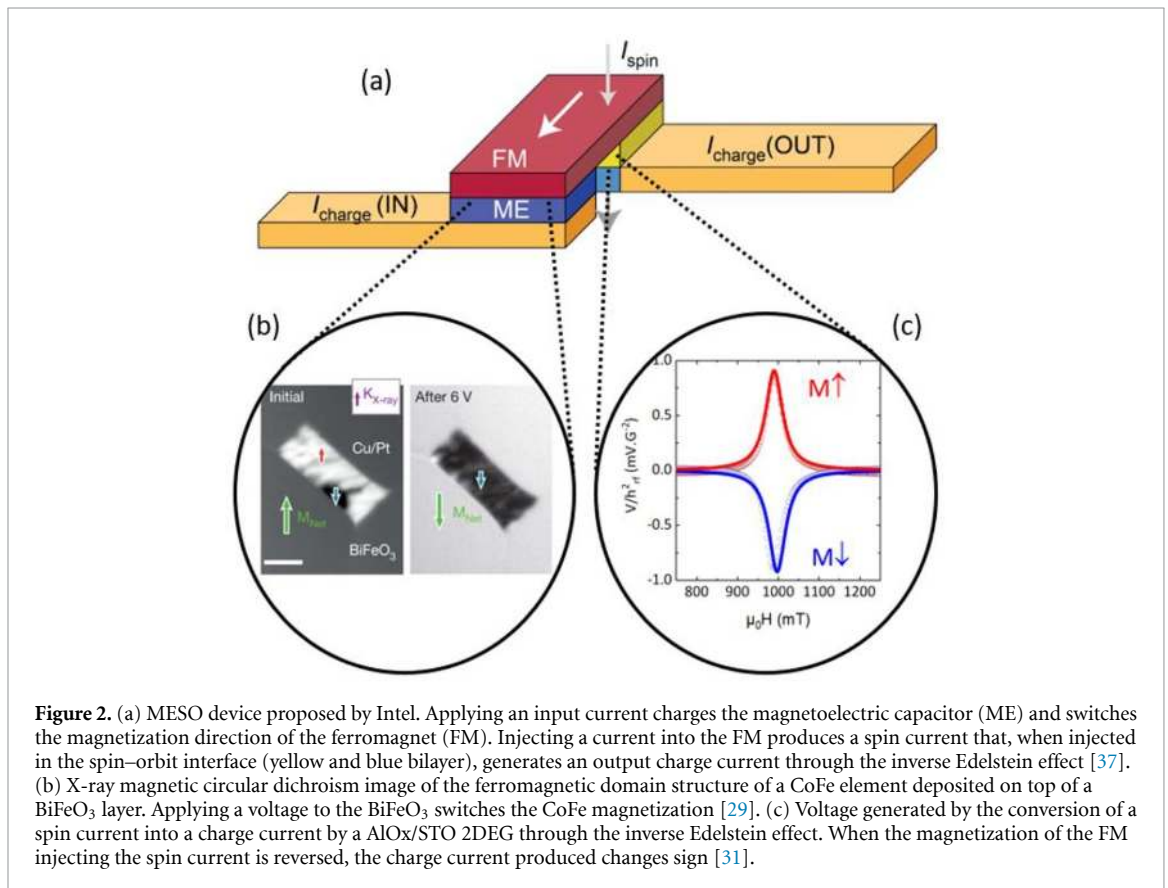


Figure 2. (a) MESA device proposed by Intel. Applying an input current charges the magneto-electric capacitor (ME) and switches the magnetization direction of the ferromagnet (FM). Injecting a current into the FM produces a spin current that, when injected in the spin-orbit interface (yellow and blue bilayer), generates an output charge current through the inverse Edelstein effect [37]. (b) X-ray magnetic circular dichroism image of the ferromagnetic domain structure of a CoFe element deposited on top of a BiFeO₃ layer. Applying a voltage to the BiFeO₃ switches the CoFe magnetization [29]. (c) Voltage generated by the conversion of a spin current into a charge current by a AlOx/STO 2DEG through the inverse Edelstein effect. When the magnetization of the FM injecting the spin current is reversed, the charge current produced changes sign [31].

The complex oxide community has also started to explore ultrafast phenomena to access transient states (including possible superconductivity at room temperature in cuprates [38]) or induce phase transitions, opening a vast new playground with many open questions.

Advances in science and technology to meet challenges

To address the challenges mentioned above a multifold strategy is required. Efforts must continue to design and synthesize new materials with high responses (e.g. a strong room-temperature multiferroic), looking beyond perovskites and towards phases that may be stabilized by epitaxy, post-growth chemical treatment, etc. We also have to identify materials combinations whose interfaces would exhibit new exotic properties (e.g. a 2DEG with Rashba SOC stronger than with STO); recent development with heavy-metal-based perovskites such as stannates and iridates are particularly promising in this direction. Another important aspect will be to synergetically exploit concurrent/competing degrees of freedom to realize novel states of matter (in the line of the ferroelectric skyrmions recently discovered see figure 1(a), but extended for instance to spin order in addition to dipole order). Combining perovskites with other quantum materials families such as transition metal dichalcogenides (TMDCs) would also bring a vast array of possibilities in terms of new physics and new devices (particularly in light of the scarcity and relatively poor stability of ferromagnets and ferroelectrics among 2DMs). Very recent progress in the preparation of complex oxide membranes will be an asset towards this goal and will also open possibilities for entirely new materials design rules inspired by the research on TBG and other moiré superlattices.

In terms of technological advances, efforts should continue to intertwine growth and characterization tools in ultra-high vacuum. *Operando* characterization is developing fast and in particular angle-resolved photoemission spectroscopy (ARPES) under piezostain or electric field has been demonstrated. As previously mentioned, ps and sub-ps physics is under intense scrutiny and should develop further to reveal hidden phases and mechanism in quantum materials based on complex oxides.

Concluding remarks

In summary, the field of oxide-based quantum matter is moving at a fast pace, which has led to several important discoveries in the most recent years (ferroelectric skyrmions, giant spin-charge conversion, superconductivity in nickelates, etc). This opens new research directions but also poses many physics questions on the conditions required to stabilize such new electronic states, the underlying mechanisms, the associated atomic, electronic and magnetic structure, etc. However, in addition to advancing the understanding the physics of complex oxides—that has paved research in condensed matter for the last 50 years—the field must also move faster towards applications (beyond the use of e.g. ferroelectrics and piezoelectrics as infrared detectors, sensors, micro-actuators or electro-optic components, all relying on bulk systems and decades-old physics). The MESO transistor recently proposed by Intel [37] and operating on multiferroics and spin-orbit materials is not only one fantastic opportunity for the field but also a broader sign that major information and communication technology companies are now ready to consider exotic materials such as complex oxides for beyond CMOS solutions.

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3. Quantum spin liquids

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Status

Quantum materials research focusses on phases of matter in which uniquely non-classical phenomena, such as quantum fluctuations, entanglement and quantized topological numbers play an essential role in establishing physical properties. Quantum spin liquids (QSLs) represent quintessential examples of such phases [39], in which the elementary degrees of freedom are the magnetic spins (qubits). Provided symmetry-breaking orders can be avoided by careful tuning of the interactions, such spins may adopt macroscopically entangled ground states, featuring e.g. topological orders and magnetic excitations with unconventional statistics. These phases are broadly referred to as QSLs.

At present, spin models represent minimal models for a wide variety of desirable phases of fundamental interest and for applications in e.g. quantum information sciences. The field spans a broad range of topics and goals, from quantum information to crystal engineering. A significant focus continues to be the unambiguous identification of a particular QSL phase in a material, which requires: (a) theoretical classification of possible QSLs, (b) focused materials searches, (c) a variety of experimental tools, and (d) interpretation of experiments aided by numerical and first-principles simulations (see figure 3).

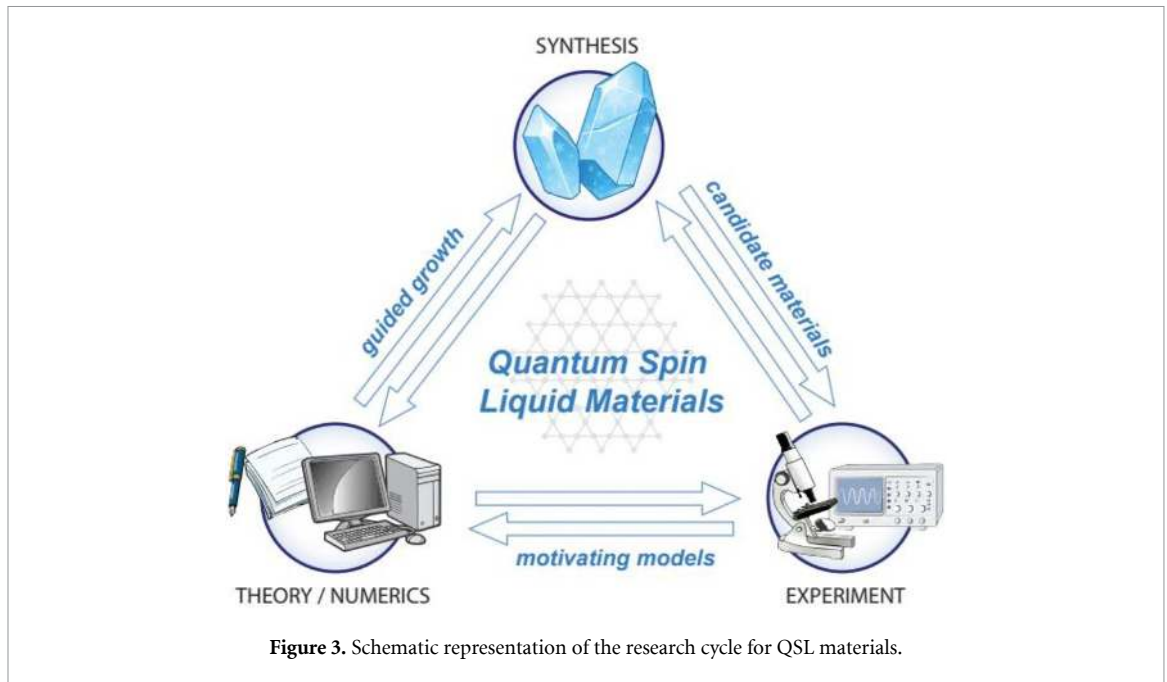
Experimental criteria in the search for QSL materials often focusses on identifying what they are not, i.e. systems where conventional order is avoided down to lowest measurable temperatures. Designing novel experimental techniques that instead directly probe their unconventional excitations or entanglement structure, continues to be a necessary target.

Traditional candidates for QSL materials are geometrically frustrated networks of spins [40] such as Kagome Herbertsmithite or triangular lattice of κ -(ET)₂Cu₂(CN)₃. However, recent years have seen an increased interest in heavy *d*- and *f*-block elements for which strong SOC induces highly anisotropic magnetic couplings. Examples include, but are not limited to, rare-earth pyrochlores [41] and various Kitaev-QSL candidates [42, 43]. These materials feature additional fluctuations driven by competition between non-commuting interactions on different bonds. However, the departure from spin-rotational invariance (and, in some cases, spin > 1/2) implies a large number of independent coupling constants are required to completely parameterize their Hamiltonians. This places increased importance on the application of a variety of experimental and *ab initio* approaches to locate given materials within broader phase diagrams.

Current and future challenges

In the discovery, characterization, and utilization of QSL materials, several challenges appear. Here, we highlight a few key challenges:

- By their nature, QSLs often occur in the vicinity of many competing phases, where relevant energy scales are artificially reduced due to frustration. This increases the importance of understanding sub-dominant effects—such as disorder—which may yield novel aspects and have a dramatic impact on experiments and the stability of given ground states [44, 45].
- Due to the complexity of magnetic Hamiltonians in modern QSL materials, estimation of the many sub-dominant couplings via experiment alone is often unfeasible; state-of-the-art *ab initio* methods are required. These methods must go beyond density-functional theory, incorporating explicit many-body treatment of spin multiplets and SOC in order to provide access to all symmetry-allowed couplings.
- In order to aid in the identification and classification of QSL materials, there is need for ‘smoking-gun’ probes of particular QSL states, as well as general experimental methodologies to probe non-local entanglement.
- Continued development of numerical methods—applicable to arbitrary quantum spin models—is needed to predict properties (particularly excitation spectra), in order to compare with experiments and characterize models.
- Regarding model development: It is generally accepted that the low-energy theory of many QSLs features emergent gauge symmetries and corresponding collective excitations. The discovery of spin models with exact solutions having a Z_2 gauge structure (such as the Kitaev’s honeycomb model [42, 43]) have bolstered this view. A challenging task is to find exactly solvable models for other phases such as U(1) spin-liquids, which have been proposed for e.g. the Kagome systems and triangular lattice organics.



- Even when exactly solvable models are found, they often have interactions that are unrealistic for real materials. Identification of realistic spin models exhibiting given ground states—and microscopic conditions for engineering them in real materials—therefore continues to be a significant focus.
- Finally, in the continued search for new QSL materials, a better understanding of how to tune materials towards desired parameter regimes is of continued interest. Various approaches are being explored, including combinations of chemical crystal engineering, physical pressure or strain, and exfoliation of 2DMs.

Advances in science and technology to meet challenges

From the experimental perspective, development of novel measurements that provide conclusive evidence of a QSL is a crucial consideration. For example, the observation of quantized thermal Hall response in a magnetic insulator represents a nearly unique signature of a chiral QSL, although better understanding of the role of phonons in these experiments is important for their interpretation [46]. Similarly, non-linear spectroscopies probing higher order spin correlation functions, such as resonant inelastic x-ray scattering, may provide more direct probes of specific excitations in QSLs if resolution can be continuously improved. To provide a measurement of non-local entanglement, spectroscopies employing multiple entangled photons is also an interesting future consideration. Similarly, the realization of QSL-equivalent states in cold-atom experiments may provide access to additional modes of measurement.

From the perspective of new material searches, finer chemical control of disorder is an ever-present target. For understanding the effects of disorder, strain, pressure, further development of *ab initio* structure predictions is likely to play an increasingly prominent role.

From the modelling perspective, adapting various numerical many-body methods to treat the lower-symmetry interactions in *d*- and *f*-block materials is highly desirable. For the calculation of dynamical correlation functions, the extension of traditional ground-state methods has proved valuable, e.g. time-dependent density matrix renormalization group and variational Monte Carlo techniques [47]. Advancements in the efficient representations of ground- and excited-state wavefunctions in 2D and 3D models, through e.g. tensor-network states, or machine-learning inspired forms [48], will no-doubt aid these approaches.

Finally, one of the motivations in the search for QSLs is the utilization of their non-trivial excitations to perform quantum computations or store quantum information. If such technologies are to be realized, they will eventually require protocols to experimentally create and manipulate such excitations.

Concluding remarks

QSLs are very exciting and, at the same time, elusive states of matter. In particular, the explosion of interest in topological quantum matter has coincided with the discovery of many spin models of fundamental interest, from Kitaev's Toric code, to fracton X-Cube models. While these models serve as an inspiration, conclusive experimental demonstrations of many predicted phases remain rare. This elusivity is likely due to a combination of (a) rarity of QSL phases in realistic phase diagrams, (b) sensitivity of QSLs to sub-dominant

perturbations such as disorder, and (c) lack of ‘smoking-gun’ experiments to uniquely identify the ground state of candidate materials. Given significant and steady progress over the years—from the conception of QSLs, to the discovery of realistic candidate materials—it seems inevitable that these challenges will be met.

Acknowledgments

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4. Twisted 2D layered crystals

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Status

When repetitive lattice structures are overlaid against each other, a new superimposed periodic lattice, called the moiré pattern, emerges. Recent progress in stacking 2DMs enables the atomic scale moiré patterning. Among the various possible atomic scale moiré lattices with 2DMs, TBG shown in figure 4(a), a single layer graphene on top of the other with a rotational stacking fault, has attracted considerable attention. The size of moiré unit cell of TBG is inversely proportional to the twist angle as shown in figure 4(b) and the Fermi velocity at the Dirac point decreases with lowering the twist angle. Specially, for a certain set of angles near 1 degree called magic angles, the velocity is strongly reduced, realizing flat bands [1, 49, 50]. A set of experiments [18, 19] exploring the flat bands in TBGs with a magic angle has ignited worldwide research activities in pursuit of new states of matters.

The magic angle TBGs (MATBGs) are insulating thanks to Mott insulating mechanism while a transition to a superconducting state is triggered under appropriate doping as shown in figure 5(a) [18]. This seemingly similar phase diagram in figure 5(b) with high temperature superconductors (HTCSs) poses a significant challenge to understand correlated physics related with doped Mott insulators in low dimensions [18]. Unlike HTCSs, the MATBGs can be easily doped without chemical means and be examined with various direct local probes on their bare surfaces [51]. With MATBGs, the other collective phenomena such as ferromagnetism [52] as well as topological properties [53] have been discovered. Besides TBGs, trilayer graphene [54–56] and double bilayer graphene [57, 58] with twist angles have also demonstrated their unique potentials in realizing novel quantum states.

Besides correlated physics in TBGs with small angles, there are also noteworthy physics in TBGs with large twist angles. One is a realization of effective 12-fold quasicrystalline order in TBGs with 30 degrees twist angle [59, 60] and the other is a higher-order topological insulating phase in commensurate TBGs with large twisted angles [61]. These works demonstrate that TBG with an appropriate twist angle can be a versatile platform for many interesting concepts in the 21st century condensed matter physics.

Together with graphitic materials, several new proposals and experiments for twisted geometries with other 2DMs such as TMDCs [62, 63] have been put forward, enriching the playground of flat bands systems.

Current and future challenges

Understanding the nature of insulating and superconducting phases in MATBGs is one of the important challenges in the field. The linear enhancement of resistivity in a broad range of temperature may indicate a ‘strange metal’ phase discussed in correlated materials [64] although the issue remains controversial [65, 66] and needs to be clarified. To uncover a true nature of MATBGs, it is important to describe electronic states, phonon dispersions and their interactions theoretically. Models and calculations for electronic structures [67, 68], phonon dispersions [69] and their mutual interactions [65, 66, 70] have been established quickly. However, to capture correlated physics, it has become crucial to incorporate strong interactions in future efforts.

Considering various degrees of freedom in manipulating TBGs and other twisted 2DMs, the new physics arising from quasiparticles and collective phenomena seem to be enormously diverse here. In particular, the complete quenching of kinetic energy of electrons reveals its consequences only in few physical phenomena such as superconducting phases [18, 19, 54–56] and anomalous quantum Hall effects [53] to name a few. So, more correlated topological phases can be expected. As already shown theoretically for spin-triplet superconductor in trilayer graphene [54–56], highly nontrivial superconducting and topological phases may be realizable. Since we can control the ratio between kinetic and Coulomb interaction by varying the twist angle, the twisted system could be one of textbook experimental tools for studying competing interactions in low dimensions. With other controlling knobs such as external electromagnetic fields and pressure, we also expect various strongly correlated optoelectric physics in MATBGs and in twisted TMDCs as already evidenced in simple TMDCs. Heterogeneously stacked twisted 2DMs, e.g. Boron-Nitride layers with TBG, have already demonstrated their unique merits [53–56] so that we expect more diverse phenomena from twisted 2DMs with different physical and chemical combinations.

The effective quasicrystalline order realized in a TBG with twist angle of 30 degrees also poses an important challenge in studying the relationship between lattice ordering and electron localization. Since the graphene quasicrystal displays strong localization far away from its Fermi energy [59, 60], either large amount of doping or other 2DM quasicrystals may realize the system to look for critical physics for electron localization related with low dimensional quasicrystals.

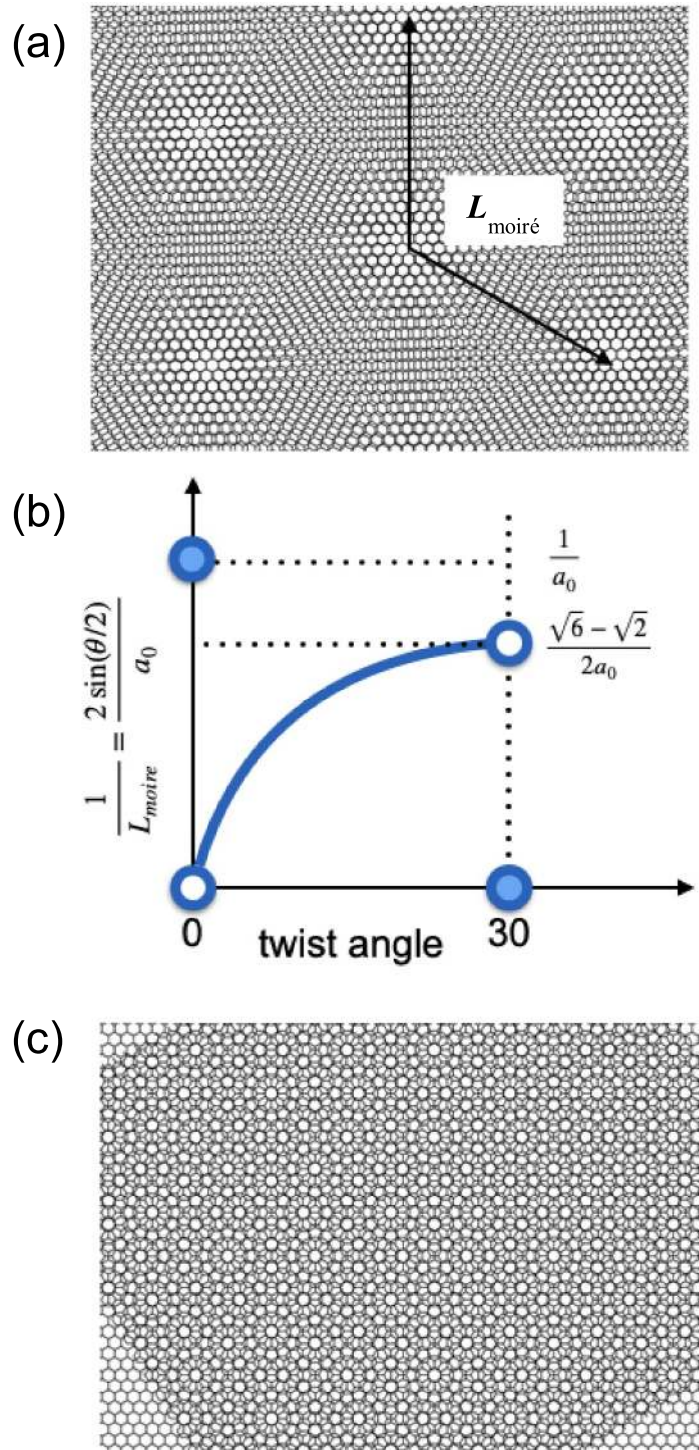


Figure 4. (a) Schematic atomic lattice structures of bilayer graphene with a rotational stacking fault. Here, a twist angle between top and bottom layer is 3 degrees. Moiré lattice with a moiré unit vector of $L_{\text{moiré}}$ much larger than graphene atomic lattice of a_0 drawn with arrows. (b) A relationship between twist angle (θ) and $1/L_{\text{moiré}} = 1/|L_{\text{moiré}}| = 2 \sin(\theta/2)/a_0$. The moiré lattice vectors do not need to match the actual commensurate lattice constants for twisted system always. In case of $\theta = 0$, the size of the vector diverges (shown in empty circle) while the actual periodicity is a_0 (filled circle). At 30 degrees, a moiré lattice of its unit vector size of $(\sqrt{6} + \sqrt{2}) a_0/2$ exists (empty circle) although the system has no translational symmetry, or a diverging unitcell (filled circle). (c) The 12-fold quasicrystalline order in TBG with a twist angle of 30 degrees.

Advances in science and technology to meet challenges

Since the most MATBGs with rotational stacking faults are hitherto fabricated through a ‘tear and stick’ method [18, 19], a controllable way of placing layers with a desired twist angle is required. Some progresses have been made [71, 72] based on nanomechanical or robotic technologies. However, considering important roles of inhomogeneous twist angles in MATBGs [73], more reliable and facile methods with high device yield should be developed. Together with these specific issues for twisted structures, other technological

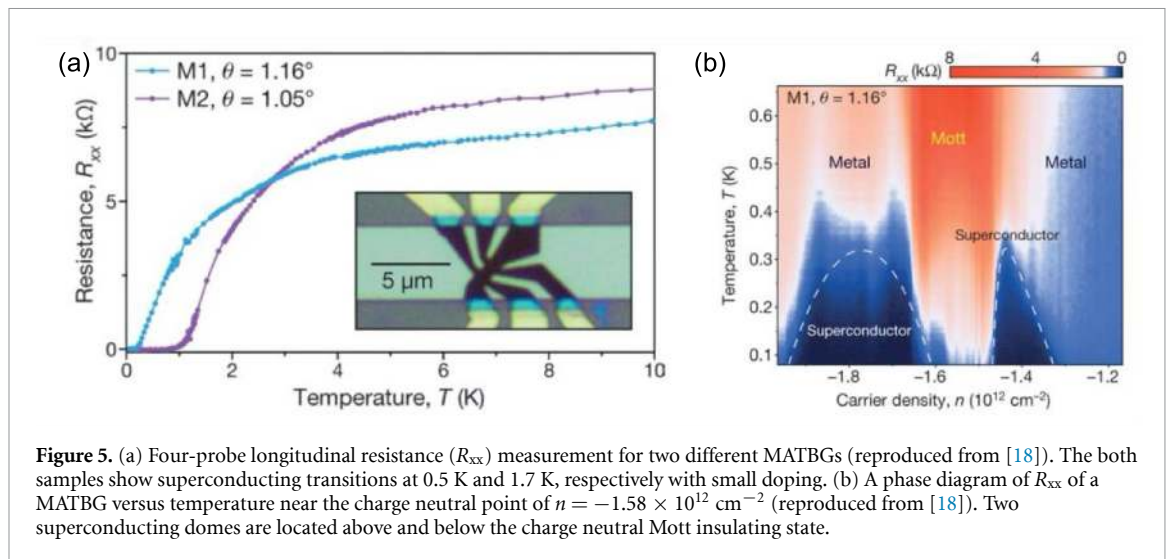


Figure 5. (a) Four-probe longitudinal resistance (R_{xx}) measurement for two different MATBGs (reproduced from [18]). The both samples show superconducting transitions at 0.5 K and 1.7 K, respectively with small doping. (b) A phase diagram of R_{xx} of a MATBG versus temperature near the charge neutral point of $n = -1.58 \times 10^{12} \text{ cm}^{-2}$ (reproduced from [18]). Two superconducting domes are located above and below the charge neutral Mott insulating state.

challenges that are common to all 2DM researches such as interfaces between 2DM and 3D materials also should be improved.

One of the most interesting physics related with twisted geometries of homogeneously or heterogeneously stacked 2DMs are related with nearly flat bands [1, 18, 19, 49, 50, 62, 63]. So, the search towards understanding novel physics relies on the analysis of the Hubbard model in 2D where the strong local Coulomb interaction dominates over the kinetic energy between lattice sites. Almost all twisted geometries involve with two or three hexagonal lattices so that the resulting moiré superlattices realize the Hubbard model on triangular symmetry. Current models from maximally localized Wannier orbitals constructed on flat bands point to interesting non-local or extended Hubbard Coulomb interactions and multiplet structures [67, 68]. A few experiments e.g. [51] already reveal an anomalous charge ordering related with the triangular Hubbard model. Therefore, in-depth analysis of this theoretical model with and without including the role of other quasiparticles such as phonon in TBGs [69, 70] will guide towards tailoring several new phases with distinct topological properties [51–58].

Considering the vast expansion of available 2DMs with different characteristics, the current set of examples for twisted 2DMs may actually just be the tip of iceberg [62–64]. To explore almost limitless combinations for twisted heterostructures, experimental techniques for a precise angle control between different 2DMs are crucially needed, together with development of the theoretical and computational machineries to describe interlayer interactions between incommensurate heterogenous lattices and the more sophisticated low energy theories based on them. Being similar with small angle twisted 2DMs, for quasicrystalline ordering, the precise angle of 30 degrees between the hexagonal layers are required so that practical techniques of building systems onto suitable substrates need to be developed beyond currently highly complicated approaches which limit the fabrication to very few devices [59, 60].

Concluding remarks

The field of physics and materials sciences on twisted layered structures of 2DMs is very rapidly growing. It already provides us intriguing parallelism between phase diagrams of MATBGs and HTCSSs. They also demonstrated several novel emergent collective phenomena of combined systems that are not characteristics of individual layers. So, the twisted 2DMs will soon become a new viable system for strongly correlated physics in low dimensions. Considering its very early stages in developments, we expect that the field will diversify itself by using various different 2DMs and that related science and technology for both fundamental researches and technological applications will thrive in very near future.

Acknowledgments

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5. Cuprate superconductors

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Status

Superconductivity in copper oxides called ‘cuprates’ was discovered in 1986. In the three decades that followed, cuprates emerged as perhaps the most remarkable and enigmatic quantum materials, with striking discoveries being made up to this day. In the first decade (1986–1997), the intensive search through hundreds of different ways to stack CuO_2 planes together with intervening layers led to a rapid increase in the superconducting transition temperature T_c , which reached its current maximal value of 133 K in 1993—still the record today for the highest T_c at ambient pressure. Two major achievements of this first decade are the conclusive demonstration that the superconducting order parameter of cuprates has d -wave symmetry [74], and the discovery of ‘stripe order’, a density-wave state of intertwined spin and charge modulations [75], which coexists and competes with superconductivity.

In the second decade (1998–2008), it became clear that at the centre of the cuprate phase diagram lies a mysterious phase called ‘the pseudogap phase’ (figure 6), whose properties have since been the focus of intense scrutiny. As the temperature is reduced below the pseudogap temperature T^* , a partial gap opens in the spectral weight for wavevectors $(\pm\pi, 0)$ and $(0, \pm\pi)$ —as detected by ARPES [76], for example—and the density of states drops dramatically—as detected in the specific heat [77], for example. The nature of the pseudogap phase is still a matter of active debate today. Numerical solutions of the Hubbard model obtain a pseudogap from strong correlations without breaking any symmetry [78], but there are proposals for a state that does break symmetry—for example, a state of current loop order that breaks time-reversal but not translational symmetry [79].

A fundamental question is: what is the Fermi surface in the pseudogap phase (at $T = 0$)? Outside the pseudogap phase, at high doping ($p > p^*$), angle-dependent magneto-resistance (ADMR) [80], ARPES [81] and quantum oscillations [82] in $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta}$ (Tl2201) with $p \sim 0.3$ all detect a large hole-like cylinder containing $n = 1 + p$ holes per Cu, consistent with band structure calculations. Inside the pseudogap phase ($p < p^*$), ARPES sees a breaking up of that large Fermi surface, with only disconnected Fermi arcs remaining in the nodal $(\pm\pi, \pm\pi)$ directions of the Brillouin zone [76]. By contrast, quantum oscillations detected in YBCO at $p \sim 0.1$ reveal a coherent and closed Fermi surface at low temperature ($T < 10$ K), once superconductivity has been removed by application of a magnetic field [83].

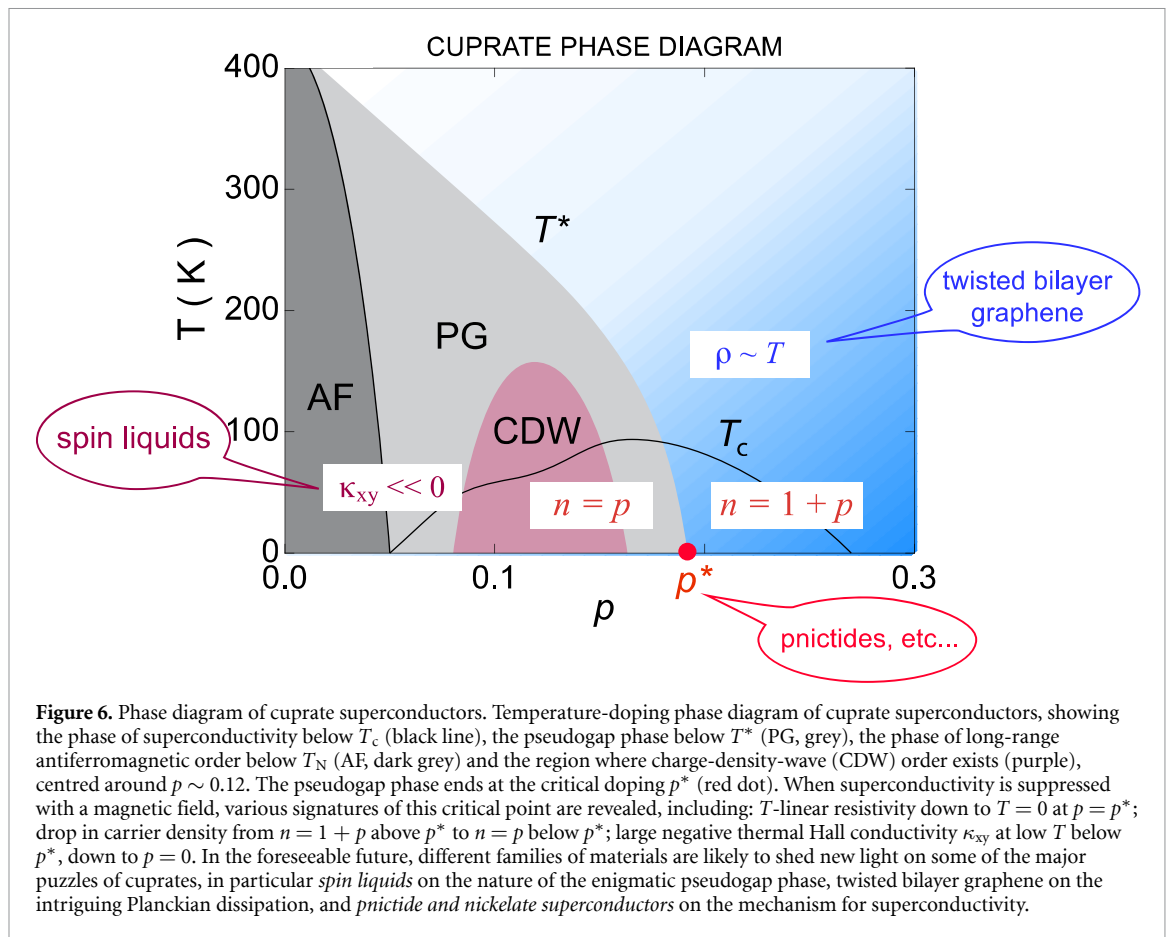
In the third decade (2009–2019), charge order was discovered in YBCO by NMR [84] and then observed by x-ray diffraction [85, 86], but without spin order, showing that spin and charge modulations do not necessarily come together. The additional periodicity associated with charge order, which breaks translational symmetry and therefore reconstructs the Fermi surface, provides a natural mechanism for the electron-like Fermi pocket seen in quantum oscillations over the same doping range ($0.08 < p < 0.16$). The fact that this range ends before the critical doping p^* at which the pseudogap phase ends shows that the two phases are distinct (figure 6). High-field Hall measurements reveal a rapid change in the carrier density, from $n = 1 + p$ above p^* to $n = p$ below p^* [87]. STM measurements using quasiparticle interference deduce a Fermi surface that goes abruptly from arcs below p^* to a full circle above p^* [88]. Whether the actual Fermi surface just below p^* —in the pure pseudogap phase without charge order—consists in fact of small closed hole pockets at nodal positions that contain p holes per Cu is a key open question.

Just above p^* , the resistivity of cuprates exhibits a strikingly linear temperature dependence down to the lowest temperatures [89, 90]. The microscopic mechanism responsible for this phenomenon, also observed in heavy-fermion metals, pnictide and organic superconductors [91], for example, stands today as one of the major puzzles in condensed-matter physics.

Current and future challenges

In 2020, several challenges are presented to us by cuprate superconductors [92, 93]. The obvious practical one is how to increase T_c . A second challenge is the perfect T -linear resistivity, seen in what are sometimes called ‘strange metals’—because they do not exhibit the standard T^2 dependence expected of Fermi liquid theory. It was recently shown that the slope of the T -linear dependence in cuprates satisfies the so-called ‘Planckian limit’ [94], whereby the inelastic scattering time is given by Planck’s constant divided by thermal energy, i.e. $\tau = \hbar/k_B T$ —as indeed it does in other materials [95]. How does this Planckian dissipation work?

A third and broad challenge is to elucidate the nature of the pseudogap phase. A first aspect is its critical point at p^* . Whereas most physical properties of cuprates exhibit a smooth crossover as a function of



temperature (through T^*), the change in carrier density as a function of doping (through p^*) is rather sharp [93]. Is this a quantum critical point, akin to that seen in organic [96], heavy-fermion [97] or pnictide [98] superconductors? In the phase diagrams of these three families of materials, a phase of long-range antiferromagnetic order is suppressed by some tuning parameter like pressure or concentration and a dome of superconductivity forms around the quantum critical point—suggesting a common pairing mechanism [99]. In cuprates, recent specific heat measurements find the same thermodynamic signatures of quantum criticality as those seen in heavy-fermion and pnictide superconductors [100]. But in cuprates, there is no long-range antiferromagnetic order near p^* ! Is it possible that short-range magnetic order is sufficient to produce the same signatures? If translational symmetry is not broken on a long range, does the change of carrier density necessarily imply a topological order [101]? Could the critical point be weakly first-order, as obtained in some Hubbard model calculations [102]?

A second aspect is the Fermi surface associated with the low carrier density $n = p$ below p^* . What is it? A third aspect is the various indications of broken symmetries [92, 93], such as time reversal, inversion, and rotation. How can we make sense of these?

Advances

The maximal T_c in cuprates has not moved since 1993, and insights from new materials would be useful. In 2008, the discovery of superconductivity in iron-based superconductors certainly showed that a high T_c was possible in other materials (up to 55 K)—the pairing in this case being most likely associated with antiferromagnetic spin fluctuations. A possible avenue of investigation is the role of phonons, which could further enhance T_c , as proposed for monolayer FeSe films [103]. In 2018, the striking discovery of superconductivity in twisted bilayer graphene [18] provides an entirely different context for pairing, with T_c values even higher than in cuprates when measured relative to the Fermi temperature (see Section 4). Another relevant discovery, made in 2019, is superconductivity in nickel oxides [104]. The comparison of cuprates to these three different superconductors is sure to be instructive.

Progress on the subject of Planckian dissipation would require having more direct measurements of the scattering time—for example via optical studies or ADMR. The recent report of T -linear resistivity with a Planckian slope in twisted bilayer graphene [57] provides a great platform for controlled studies of this phenomenon.

For the pseudogap phase, one of the most decisive measurements would be to see quantum oscillations in the pure phase (without charge order). In the cleanest materials like YBCO, $\text{HgBa}_2\text{CuO}_{4+\delta}$ and Tl2201, all with a high maximal T_c (~ 90 K), the magnetic fields necessary to suppress superconductivity down to $T \sim 1$ K are in excess of 100 T [105]—requiring new techniques for detection in ultra-high fields. Seeing oscillations with a frequency $F = p \Phi_0/2$ —coming most naturally from nodal hole pockets with a total carrier density p —would go a long way to establishing the wavevector (π, π) as a fundamental organizing principle of the pseudogap phase.

Further advances in computational methods would help tighten the connection between the Hubbard model and the real cuprates—ideally by being able to resolve the expected Fermi surface in the pseudogap phase—and other theories of the pseudogap phase—for example the $\text{SU}(2)$ gauge theory of fluctuating antiferromagnetism, with its topologically ordered Higgs phase [106].

The recent observation of a large thermal Hall effect in the pseudogap phase of cuprates [107] raises an entirely new question: by what mechanism can the pseudogap phase confer chirality to neutral excitations? The same question is now being asked in the context of spin liquids, insulating materials where magnetic order is frustrated by the structure, in favour of new states of quantum matter that are expected to potentially harbor new excitations such as spinons or Majorana modes, whose presence may be detectable by the thermal Hall effect [108].

Concluding remarks

A promising roadmap for tackling the biggest questions about cuprate superconductors—maximal T_c , Planckian dissipation, pseudogap phase—is to explore connections with other materials, in particular iron-based and nickelate superconductors, twisted bilayer graphene and spin liquids.

Acknowledgments

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6. Ultrathin layered superconductors

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Status

Superconductivity in two dimensions has fascinated the scientific community since the late 1930s, but due to the many surfaces and interfaces of a 2D system resulting in the tendency for structural and chemical disorder, early experimental work was restricted to the investigation of amorphous or granular thin films of metals and alloys. This work allowed the study of important properties of the superconducting state independent of the crystal orientation and structure. It was found, for example, that the angular dependence of the upper critical magnetic field exhibits a peak-like response if the magnetic field is parallel to the thin film. This was subsequently explained by a phenomenological theory based on the Ginzburg–Landau model and is considered a signature feature of 2D superconductivity [109].

Recent technological advances, such as molecular beam epitaxy (MBE), pulsed laser deposition, electric double layer transistors, and mechanical exfoliation allow the fabrication of highly crystalline and atomically-thin samples, and experimental progress with techniques such as scanning tunnelling spectroscopy and angle-resolved photoemission spectroscopy enable researchers to investigate materials' properties that are intimately linked to their crystal structure.

On the theoretical side, the availability of high-performance computing clusters, in combination with advances in *ab-initio* calculations enable researchers to quantitatively reproduce and even predict quantities like the superconducting critical temperature T_c .

Particular efforts were made to shed light on quantum phase transitions, as for example between the insulating and superconducting state, or between metallic CDW phases and superconductivity, as well as Ising-, interface-, and topological superconductivity [109, 110]. Of particular interest in this respect are TMDCs, layered materials whose layers are held together by weak vdW forces. This allows the exfoliation down to the monolayer limit, making them one of the thinnest superconductors made to date (figure 7).

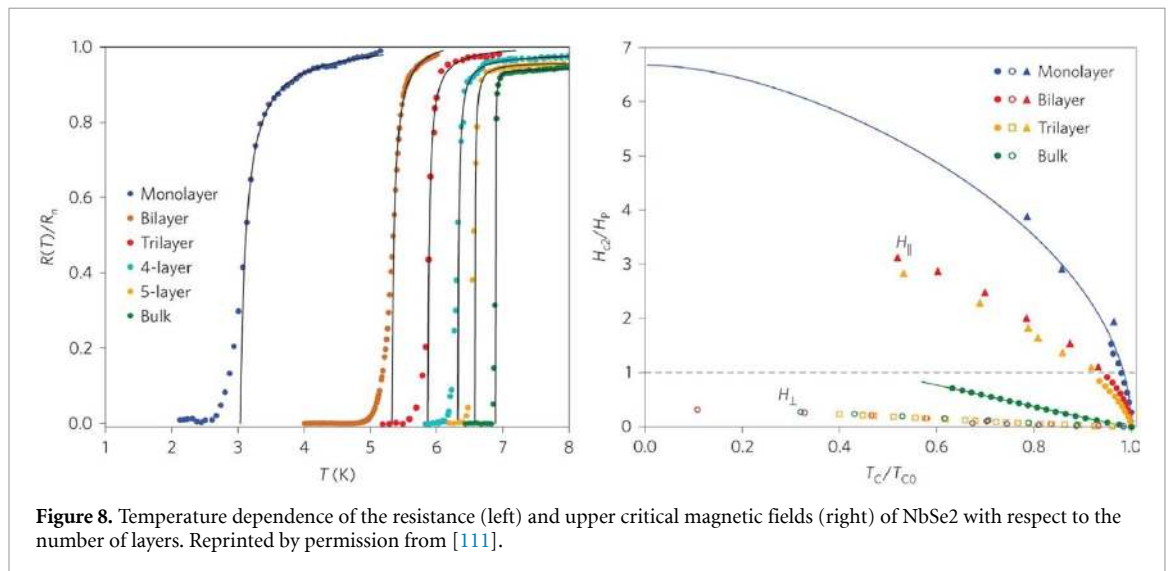
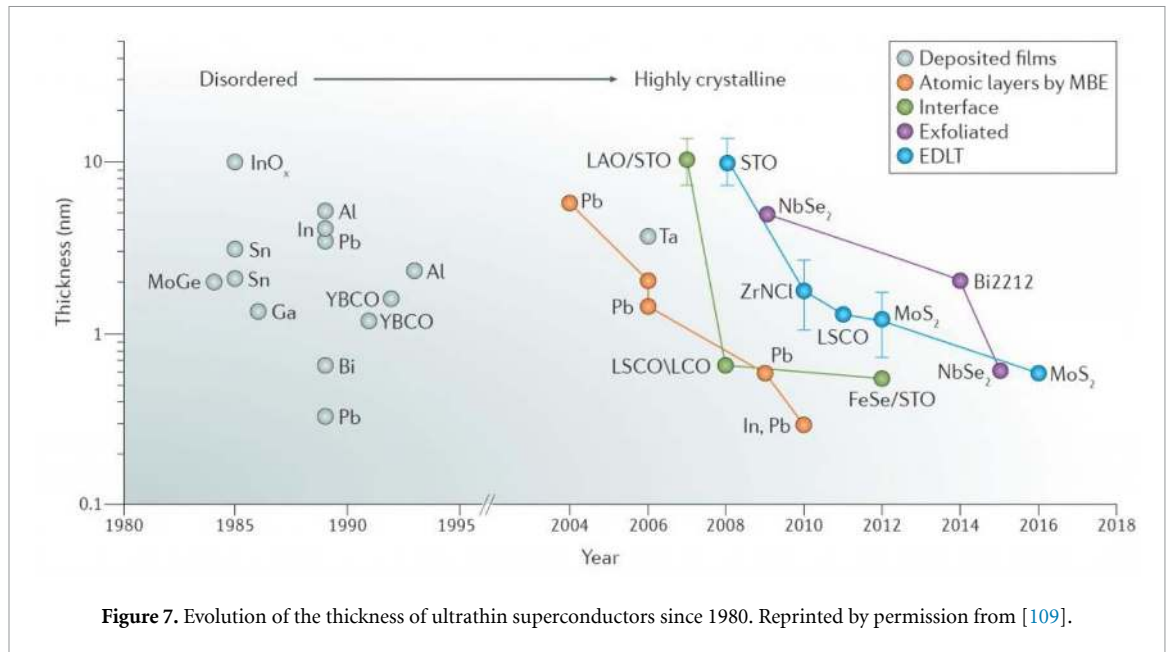
Two other fascinating examples of 2D superconductivity that we want to mention in passing are (i) monolayer FeSe on STO, featuring a T_c of ~ 65 K, compared to the bulk value of ~ 8 K, and (ii) bilayer graphene, which becomes superconducting ($T_c \approx 1.7$ K) if the two layers are twisted by the so-called 'magic angle' of about 1.1 degrees with respect to each other [18, 109, 110].

Current and future challenges

TMDs have attracted great research interest as their superconducting phase often coexists with CDW phases. NbSe₂, for example, exhibits a CDW phase below 33 K and is superconducting with a $T_c \sim 7$ K in the bulk. When thinned down, T_c decreases monotonously reaching a $T_c \sim 2$ K in the single-layer limit (figure 8, left) [109–111]. The existence of a CDW for the monolayer at a higher T_{CDW} than in the bulk has been predicted theoretically [112], and while a CDW has been observed experimentally, studies are in disagreement at which temperature T_{CDW} this phase sets in. Interestingly, a recent theoretical study predicts that both T_c and T_{CDW} increase in the closely related TaSe₂ when thinned down from bulk to monolayer [113]. Experimentally, a strengthened CDW and increasing superconductivity were observed in few-layer samples. If SC survives in the monolayer limit of TaSe₂, and why SC reacts differently in different TMD materials when thinned down are just two questions that need to be investigated further.

One of the most intriguing features of SC in ultrathin TMDs is the fact that it survives huge in-plane magnetic fields, factors of 5 and larger than the corresponding Pauli paramagnetic limit (figure 8, right) [111, 114]. A possible explanation for this behaviour is based on strong spin–orbit interactions leading to almost perfect spin splitting in certain valleys of the Brillouin zone. In the superconducting phase, the Cooper pairs are formed between these valleys, resulting in an internal magnetic field protecting SC [109, 111]. A recent study extended this concept of *Ising superconductivity* to certain centrosymmetric 2DMs, opening up a very interesting path for further research [115].

Within the versatile class of TMDs one can also find TIs. Monolayer WTe₂, a quantum spin Hall (QSH) insulator, can be reversibly tuned to become superconducting using the electrostatic field effect [116]. The proximity of a topological insulating state to a superconducting phase offers many new and interesting research directions. For one, it has not yet been clarified whether the superconducting state itself is topologically nontrivial or not, and it would be fascinating to investigate Majorana modes within these materials.



Advances in science and technology to meet challenges

Recent theoretical improvements allow the description of the superconducting phase fully *ab initio* and to look at quantities like the superconducting gap function or the electron-phonon coupling resolved by electron energy bands and momentum, offering unprecedented insight into the origins of SC in TMDs [117]. To improve the theoretical description further, it would be important to include anharmonic and non-adiabatic effects, as the superconducting phase in these materials appears in close vicinity to quantum phase transitions and lattice instabilities [112, 113, 117]. Also, in order to be able to describe concepts like Ising superconductivity, spin-polarization needs to be taken into account in the calculations.

With respect to superconductivity in the vicinity of nontrivial topology, fascinating new phases and states might yet to be unravelled, possibly requiring the consideration of new models to describe SC there. A recent theoretical work, for example, proposes a way to realize Majorana fermions in monolayer NbSe₂ and TaS₂, employing magnetic fields higher than the Pauli limit, but lower than the in-plane critical field required to turn them into nodal topological superconductors [118].

At this point it should also be noted that in most experimental setups, the ultrathin TMD samples are placed on a substrate and protected by a capping layer, thereby representing a complex layered heterostructure. Great care has to be taken to attribute any measured physical quantity or phenomenon to its origin within this heterostructure. On the other hand, a lot of theoretical work is based on freestanding mono- and few-layers to keep computational costs to a minimum. While this allows for investigating effects confined to the ultrathin layer, it does not quite represent most experimental setups, as interfaces can have

important influences on quantities like electron–phonon interaction and superconductivity. One of the key advances in the next few years should therefore be to improve our understanding of interlayer physics with respect to quantum phase transitions and superconductivity in particular. On the theoretical side, this means to consider large supercells and heterostructures to better capture the experimental setup.

Concluding remarks

Ultrathin layered superconductors are a highly topical field in condensed matter research and the progress that has been made recently is considerable. Apart from proving that robust superconductivity can indeed exist in 2D and verifying concepts like the Berezinskii–Kosterlitz–Thouless transition and quantum Griffiths singularity, researchers have found ways to induce (topological) insulator to superconductor transitions, unravel Ising pairing, and shed light on the coexistence of CDW order and superconductivity, to name just a few milestones [109, 110]. It is to be expected that this research pace will even further increase with prospects of finding topologically nontrivial superconductivity, the observation and manipulation of Majorana zero modes (MZMs), and possibly new high- T_c superconductors, to name just a few examples, along this highly fascinating road of research.

Acknowledgments

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7. Topological insulators

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Status

First introduced in 2005 by Kane and Mele, TIs constitute a new topological phase driven by SOC and symmetries, yielding a bulk insulator with spin-polarised 'topologically protected' conducting boundary states (see review [119] and references therein). 2D-TIs exhibit the QSH effect, i.e. a pair of counter-propagating spin-polarised edge states, responsible for quantized conductance at zero magnetic field, as observed in HgTe QWs [119] and monolayer WTe₂ [12]. 3D-TIs sustain massless topological surface states (TSS) with a peculiar spin-momentum locking. Interestingly, the TI class of materials includes a broad range of vdW systems, such as the 3D-tetradymites [(Bi,Sb)₂(Se,Te)₃] family that exhibit robust insulating bandgaps. Although angle-resolved photoemission spectroscopy [119], magneto-transport and magneto-optic techniques have provided invaluable insights into their boundary states, the current challenges reside in exploiting their superior transport properties for emerging topological electronics and spintronics, which is the focus of this roadmap section.

QSH is a promising platform for spin-to-charge conversion and superconducting topological junctions. In particular, TIs in proximity with superconductors exhibit electronic states that support Majorana fermions, a phenomenon that opens new avenues for topological quantum computation [120]. However, conductance quantization (figure 9(a)) suffers from limited spatial robustness, suggesting that topological protection via time-reversal symmetry (TRS) remains fragile. TSS transport in 3D-TIs is more robust, especially in buried topological heterojunctions. It is also quite rich as Volkov and Pankratov, who anticipated TSS back in 1985, predicted the existence of massive surface states in smooth heterojunctions (VPs), both subject to a relativistic field-effect limiting Dirac screening [121].

Observation of unique quantum phenomena in TIs requires TRS to be broken, as well as introduction of an exchange gap. In fact, breaking TRS in 2D and 3D TIs through magnetic doping, as in Cr- and V-doped (Bi,Sb)₂Te₃, has led to the advent of magnetic TI (MTIs) that manifest robust quantum anomalous Hall (QAH) effect [16, 122] (figure 9(b)), topological magnetoelectric (TME) effect [123], and constitute a platform for axion electrodynamics. Tailoring and engineering of MTIs and their heterostructures have been also successful in this respect. Exploitation of the TSS, spin texture and strong SOC in devices incorporating TIs has proven their potential for spintronic applications.

Current and future challenges

The relative fragility of QSH quantization in TIs remains unsolved. Today, improved nanofabrication methods comprise cleaner etching techniques that enable the realization of smooth edges where robust QSH transport and superconducting topological junctions in HgTe-QWs at the micrometer scale are observed [124]. Despite the advances this achievement entails, it is not yet comparable to the high-precision QAH quantization reported in 100 μm -long Cr-doped (Bi,Sb)₂Te₃ Hall bars [125]. Even if further progress is expected on the technological side, the marked contrast between QSH and QAH quantization raises basic physics questions on the absolute robustness of TRS protection. Possible routes may rely on the combined effects of disorder and interactions [126], or decoherence by coupling to the environment bath which control the irreversible decay toward thermodynamic equilibrium. Engineering this environment is a key challenge that requires a better knowledge of bulk electronic but also bosonic excitations, such as phonons, plasmons, polaritons, magnons, and the still elusive axion electromagnetic modes.

Similarly, new routes and concepts are required in order to improve the properties of MTIs. The first intrinsic MTI, the layered antiferromagnet MnBi₂Te₄, was recently discovered, where both QAH [16] and axion [123] insulator states occur depending on the parity of the number of layers (figure 10). Notwithstanding, the low temperatures (<2 K) at which these and related quantum phenomena are observed in this material, as well as in magnetically-doped TIs, makes it challenging to incorporate them in devices with practical applications. Reducing disorder in the exchange gap is believed to widen the temperature range in which quantum phenomena manifest in these systems. Alternative approaches take advantage of/make use of proximity effects in magnetic heterostructures incorporating TIs to pursue QAH effects, as well as to use chiral edge modes to electrically control the magnetization, or vice versa, exploiting spintronic effects such as SOTs.

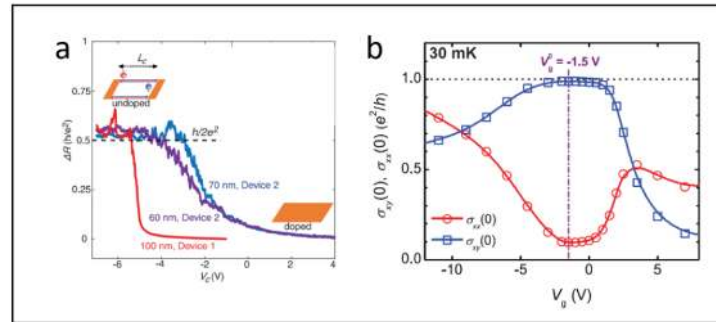


Figure 9. Examples of conductance quantization in TIs. (a) The quantum spin Hall (QSH) quantization (in units of $2e^2/h$) in the insulating bandgap of single layer WTe_2 devices is quite fragile and vanishes at the micrometre scale. QSH is observed for two devices with different channel length (100 and 60–70 nm) and WTe_2 width [12]. (b) Sheet conductance at zero magnetic field in the longitudinal, $\sigma_{xx}(0)$, and transverse (Hall, $\sigma_{xy}(0)$) geometries in the insulating bandgap of Cr-doped $(\text{Bi,Sb})_2\text{Te}_3$. The distinct plateau with the quantized value e^2/h observed at zero magnetic field is characteristic of the quantum anomalous Hall (QAH) effect. Panel (a) reproduced from [12] and panel (b) from [122].

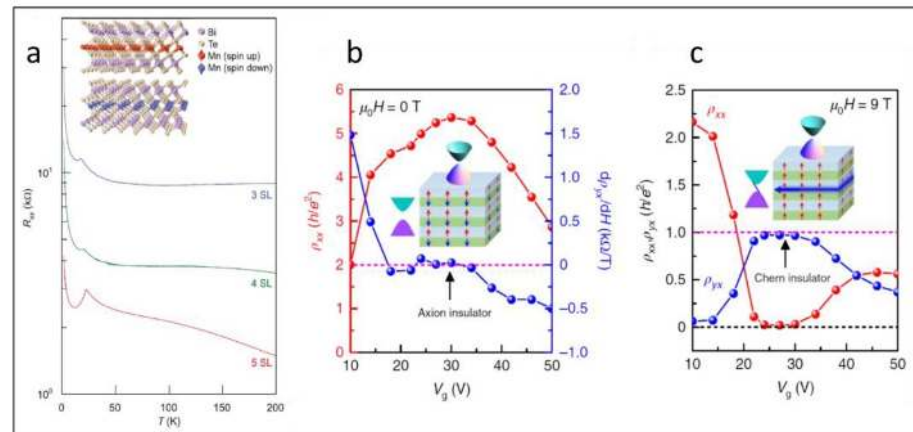


Figure 10. (a) Temperature dependent sample resistance of few-layer MnBi_2Te_4 . The antiferromagnetic transition manifests as a resistance peak in the three-, four-, and five-layer samples. Inset shows the layered crystal structure of MnBi_2Te_4 in the antiferromagnetic state. The spins of Mn^{2+} ions order ferromagnetically within a layer, whereas neighbouring layers couple antiferromagnetically with an out-of-plane magnetocrystalline anisotropy. Gate-dependent resistance of a six-layer MnBi_2Te_4 exhibits (b) axion and (c) Chern insulator (QAH) states. Insets in (b) and (c) illustrate of the magnetic order and electronic structure of such states. Panel (a) adapted from [16] and panels (b) and (c) reproduced from [123].

Both in the case of MTIs and non-MTIs, along with their heterostructures, further theoretical studies and experimental investigations are needed to take up the challenge and fulfil the promises of topological electronics and spintronics. From the experimental point of view, the versatility of vdW-TIs offers a unique platform for topological science that is still at its infancy. In terms of theoretical advances, models of interacting TIs could provide relevant information to experimentalists, and predict the emergence of even more exotic states of matter.

Advances in science and technology to meet challenges

TI physics and technology has not reached the readiness level to envision the building up of a genuine ‘topotronics’ foundry. If narrow-bandgap semiconducting TIs (CdHgTe , PbSnTe) are produced at the wafer scale with high mobility, it is not yet the case of medium bandgap vdW-TIs. In the near future, the latter will largely benefit from the intense efforts worldwide to realize large scale, high-quality films and heterostructures with controlled chemical doping. On the device side, a better understanding of the specific field effect in TIs is needed because of the coexistence of trivial and topological carriers. It would deserve a new compendium on the physics of topological semiconducting devices. It is also very desirable to build a comprehensive database on TI-material excitations, in complement to the recent catalogue of high-quality topological crystals [26, 27], as they play a crucial role in limiting finite-bias properties of topological devices. As a matter of fact, TI materials, which aim at being sensors for thermal, magnetics, far-infrared and microwave excitations, and building blocks of topological quantum computation, are primarily sensitive to their own thermal fluctuations bath. There are possibly more crystalline structures to be synthesized from

chemistry among the 3307 TI-crystals identified in [27], possibly including cleverly engineered metamaterials including twisted vdW materials. On the physics side, the role of interactions in triggering collective instabilities is worth investigating. A theoretical account of actual finite confinement lengths calls for a phenomenological approach of coexisting trivial and topological carriers in the presence of band bending.

On the experimental side, high-quality growth and fabrication of TIs and their heterostructures is currently achieved by MBE, which continues to be the best technique to produce, for instance, layered materials with superior properties than their bulk crystal counterpart. Optimized MBE grown MTIs, such as MnBi_2Te_4 and related compounds, should reduce their disorder and further increase the energy scale of the desired QAH and TME effects. More exotic quantum states may be implemented with heterostructure engineering and appropriate materials combinations. Efficient control of the TME and other spin-related phenomena is one of the main goals in spintronics and would constitute a further step towards industrial applications of TIs.

Concluding remarks

The last 15 years have been intense and very active in research and development of TI materials. Important progress has been done, but further improvements in the quantization, energy and temperature scales are required in order to achieve industrial and technological advances. The gap between fundamental research and practical applications remains open and further strategies are needed to close it. More in-depth theoretical and experimental research is required to clarify the nature and characteristics of strong SOC effects, in order to guide experiments towards more efficient and practical implementations of spin-related mechanisms.

Acknowledgments

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8. Topological semimetals

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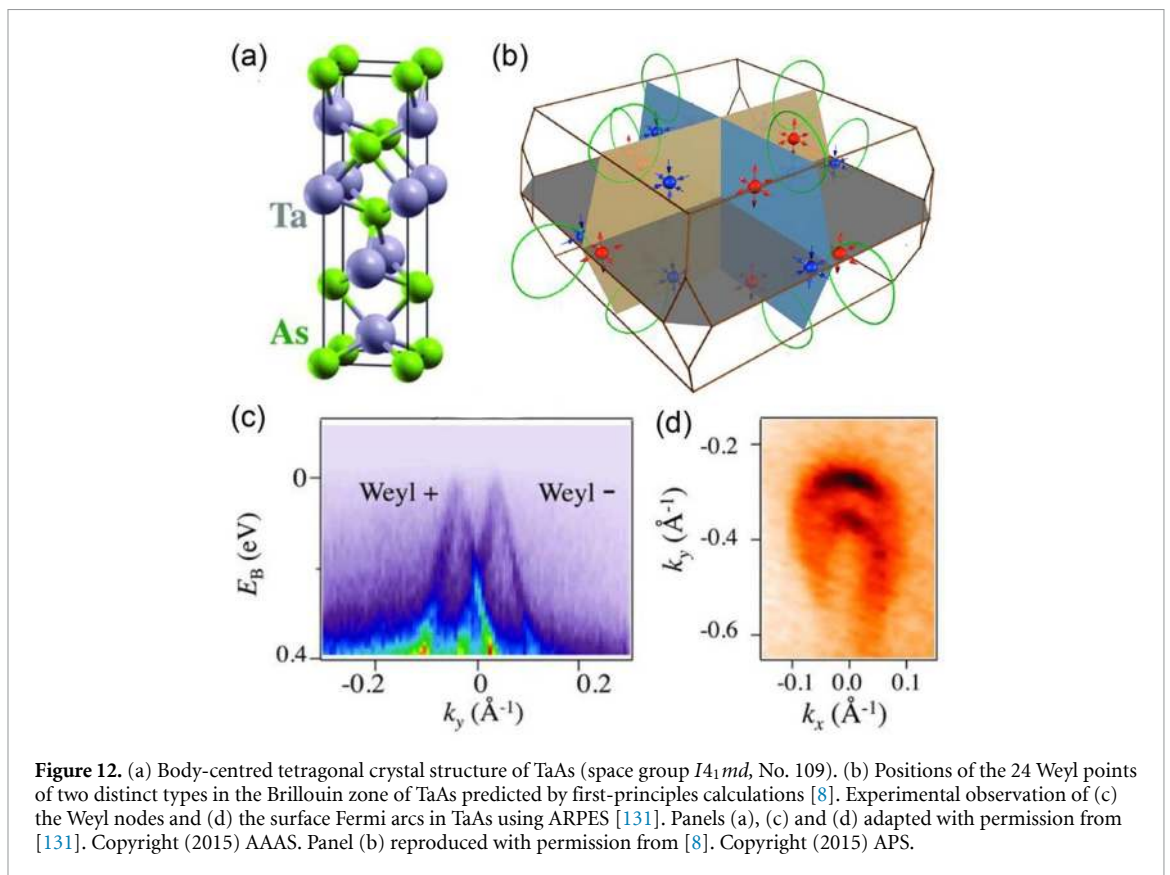
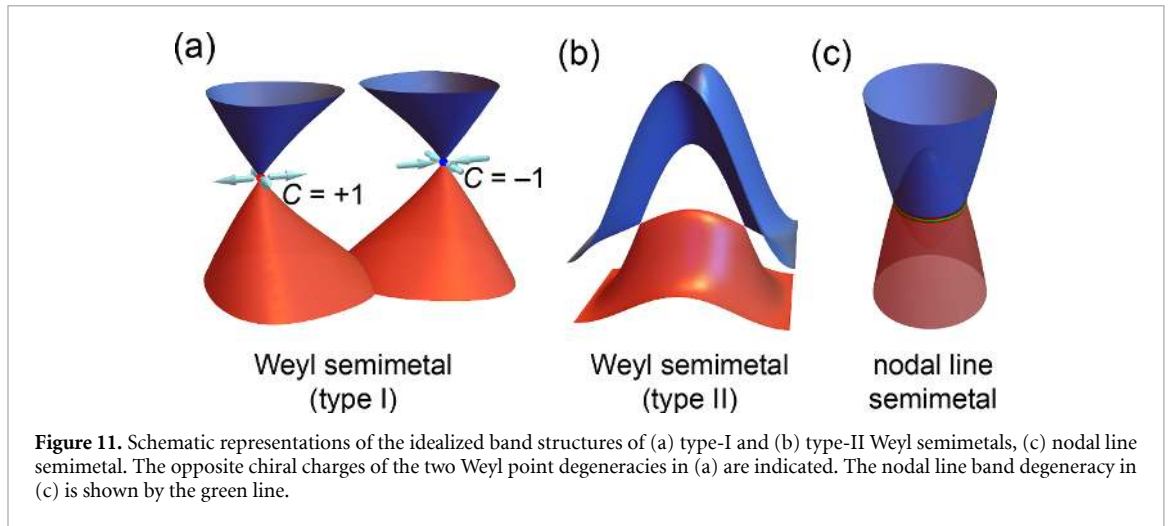
Status

The field of topological materials has seen explosive development during the past decade. While initial efforts focused on materials hosting insulating topological phases (Z_2 TIs, followed by topological crystalline insulators), it was soon realized that gapless topological phases also present rich and exciting physics [127]. The first relevant topological phase is the Dirac semimetal characterized by the point band degeneracies connecting linearly dispersing bands at the Fermi level. In these materials, which can be viewed as 3D analogues of graphene, the four-fold band degeneracies are protected by the crystalline symmetries. Two notable examples of Dirac semimetals are Na_3Bi [128] and Cd_3As_2 [129], both experimentally confirmed in 2014 following earlier theoretical predictions. Breaking inversion results in two-fold band degeneracies that are chiral, i.e. characterized by non-zero chiral charges (figure 11(a)). Materials in which such point degeneracies are isolated at the Fermi level are referred to as the Weyl semimetals [130]. First members of this broad class of topological semimetals have been discovered in the TaAs family of materials in 2015 (figure 12(a)) [8, 131]. The notion of type-II Weyl semimetals was then introduced to account for the case of strongly tilted conical band dispersion with band degeneracies representing the touching points between electron and hole Fermi surface pockets (figure 11(b)) [132]. Examples of type-II Weyl semimetals are the initially proposed ditellurides WTe_2 [132] and MoTe_2 , confirmed robust Weyl semimetals in diphosphides WP_2 and MoP_2 [133]. Band degeneracies can further extend along a line or a loop (figure 11(c)) leading to another distinct topological phase—the nodal line semimetal—with PbTaSe_2 and materials from the ZrSiS family being typical representatives. The classification of topological semimetals does not stop here now including scenarios with even more complex forms of band degeneracies, such as nodal chains, six- and eight-fold degeneracies, and novel classification schemes such as the non-Abelian band topology [134]. Likewise, the number of theoretically proposed and experimentally confirmed materials hosting these phases continues growing at a steady pace. The progress in the emerging field of topological semimetals is mostly driven by the exploration of fundamental physics, but prospective technological applications of these novel materials are also being discussed. As far the fundamental aspects are concerned, the paradigm of realizing new types of fermions as quasiparticle excitations in topological condensed matter systems establishes an interesting connection with high-energy particle physics. On the other hand, novel properties of topological semimetals are actively investigated for potential applications ranging from catalysis to topological quantum computing.

Current and future challenges

The field of topological semimetals can be regarded as nascent and shows very rapid evolution. Despite the frequently emerging new ideas, the outstanding challenges in the field have been posed since its very beginning. We can identify the following open problems:

- (a) ARPES remains the primary experimental tool for confirming the presence of a topological semimetal phase in a given ‘candidate’ material, while the predictions would typically rest on materials chemistry intuition, symmetry considerations and the results of first-principles calculations. ARPES provides direct access to topological band degeneracies in bulk band structures as well as to the surface states resulting from the corresponding bulk topological phases (figures 12(c) and (d)), e.g. Fermi arcs and drumhead states in the Weyl and nodal line semimetals, respectively. However, observing the anticipated unusual transport signatures of the topological phases, e.g. the chiral anomaly, gravitational anomaly, the planar Hall effect, etc. appears to be more challenging. Despite numerous reports in the literature, there is a growing concern regarding possible alternative explanations of these measurements, or even their reproducibility.
- (b) It would not be an exaggeration to say that theoretical predictions have been driving the progress of the field of topological semimetals. Many recent high-throughput computational surveys claim that a substantial fraction of all known crystalline materials host some kind of topological phase. This is not surprising given the fact that breaking the inversion or time-reversal symmetries, or introducing non-symmorphic symmetries, is sufficient for creating topological band degeneracies. The real challenge, however, consists in finding materials having the minimal possible number of such degeneracies isolated at the Fermi level, in correspondence to the ideal models of topological semimetals. Currently investigated materials, such as the TaAs-family Weyl semimetals, are still far from the ideal models showing very



complex arrangement of topological band degeneracies (figure 12(b)). A close dialogue between theory and experimental researchers is necessary for overcoming this challenge.

- (c) Most currently investigated topological semimetals are weakly correlated materials. It is anticipated, however, that the combination of topology and strong electron-electron interactions will open vast opportunities for discovering novel physical phenomena. Finding a convenient platform material that realizes such interplay between strong correlations and topology as well as focusing both theoretical and experimental efforts on a particular important phenomenon is a challenge that needs to be addressed in the coming years.
- (d) Currently, the progress in the emerging field of topological semimetals is largely driven by the exploration of novel physics rather than by prospective technological applications of these materials. Identifying an application domain where topological semimetals will play the role of enabling materials, finding a material that could be considered the ‘silicon’ of topological semimetals and developing device manufacturing techniques defines another challenge for this emerging field.

Advances in science and technology to meet challenges

The field of topological semimetals is still very young, but it quickly advances towards reaching maturity. It is currently flooded with a large number of proposed novel physical phenomena, different kinds of topological phases as well as candidate materials hosting them. As far as the discovery of new topological materials is concerned, ongoing developments in computational methods and software, open science initiatives and incorporation of ML techniques, accelerate the progress in the field. Further advances in this domain will soon lead to identifying the most interesting phenomena and materials, thus making scientific progress in this field more coherent and focused. One can expect that for selected topological semimetals progress in developing growth methods compatible with common device manufacturing strategies will enable exploring the technological potential of these emerging materials. First steps in this direction have already been reported [135].

Concluding remarks

The field of topological semimetals and the broader domain of topological states of matter are currently among the most rapidly expanding areas of physics. One can expect that very soon topological materials will have their own chapter in introductory condensed matter physics textbooks, at the same level as semiconductors, superconductors or magnetic materials. The grand challenge of the field, however, consists in realizing first paradigm shifting technological applications of the newly discovered physical phenomena and materials. Success in achieving this goal largely depends not only on collaborative research in theoretical and experimental physics, but also on extensive involvement of researchers in chemistry, materials science and engineering disciplines. These adjacent fields are only starting to realize the perspectives of topological materials.

Acknowledgments

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9. Quantum materials for topological devices based on Majorana modes

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Status

Majorana zero modes (MZM) are quasi-particle states that can exist at interfaces in certain classes of materials. The states are inherently non-local and the emergence of a split pair of Majorana states is a remarkable manifestation of topology, an important new paradigm in condensed matter physics with direct links to materials science [136]. The observation and manipulation of these exotic quasi-particles are of great scientific interest; for instance they do not obey ordinary (fermionic) exchange statistics.

Topological states entail schemes for realizing quantum information processing based on qubits that are in principle protected from decoherence. This advantage over other solid state qubits has not yet been demonstrated, but electrical transport experiments have shown signatures of the essential Majorana modes that potentially allow for encoding of the topologically protected qubit states.

We focus here on electronic semiconductor devices while noting that other materials have been studied e.g. by STM [136]. The Majorana modes emerge as degenerate, zero-energy states and they are predicted to exist at the ends of one-dimensional (1D) conductors in a topological superconducting state [137] (figure 13(a)). Until date most experiments have been based on III–V semiconductor nanowires (InAs, InSb) grown by vapour–liquid–solid growth (VLS) [138]. In these semiconductors spin–orbit interactions are strong and they can be readily interfaced with superconducting materials—key ingredients needed for realizing the topological state. The materials have been refined by development of hybrid materials where superconducting layers are grown directly on semiconductors *in situ*. Some elemental superconductors can be matched epitaxially to facets of semiconductor nanowires (figure 13(b)), facilitating transfer of the superconducting correlations uniformly into the semiconductor nanowire.

The first promising results were observed in two-terminal electrical measurements on nanowires, configured to allow for tunnelling spectroscopy of the electronic states in a semiconductor segment contacted by a superconductor [139]. Here, the desired MZMs were reported to appear as zero-bias peaks (ZBPs), i.e. distinct signals in electrical transport when electrons could tunnel into a Majorana state. A typical device is shown in figure 13(c). Such experiments merely indicate the existence of the MZM [140]. While other concepts such as quantum dot and Josephson effect spectroscopies have also been implemented [138, 140], none of these experiments allow to test the most profound consequence of topology, the non-Abelian exchange statistics. This would require tunable junctions between multiple 1D nanowires. This need for more complex devices has stimulated significant efforts on developing new nanostructured hybrid materials.

Current and future challenges

ZBP signals have been reported, but despite much effort there is no conclusive evidence for MZM. A braiding experiment should reveal the non-Abelian statistical properties, and at the same time could embody a first Majorana qubit. This is a challenging experiment, and currently out-of-reach due to the required device quality and complexity [141] as will be discussed below. A more accessible experiment, and a stepping-stone towards braiding, is to demonstrate correlations between two ZBP states at each side of a topological superconductor (figure 13(a)). Correlated states showing all properties as expected from MZM will provide strong indications for the existence of Majorana modes.

The challenge to be addressed for these correlation experiments is the quality of the devices. It has been argued that the ZBPs observed so far could have been induced by disorder [140]. Disorder can be present in the nanowire channel or at the semiconductor/superconductor interface. Disorder in the semiconductor channel is probably induced by the nearby surface and could be reduced by moving surface states further away by using high quality shells, or by using 2DEGs, which are pinched off to form a 1D channel. Challenge of the materials used in these studies is their large lattice constant and the inherent difficulty in finding suitable lattice-matched materials that could serve as a substrate or shell. The quality of the semiconductor/superconductor interface has been greatly improved by epitaxial growth (figure 13(b)) [142]. A new problem arising from epitaxial growth is that the semiconductor channel is ‘metallized’ by the superconductor due to the much higher density of states. A solution could be to employ a tunnel junction to tune the semiconductor/superconductor coupling. Another approach to mitigate the effect of disorder is by increasing energy scales of the topological system, which would require new materials.

Although the clearest ZBP signals have so far been obtained with bottom-up grown VLS wires, this system is not scalable towards larger circuits with complex device geometries (figure 14(a)). There is a great

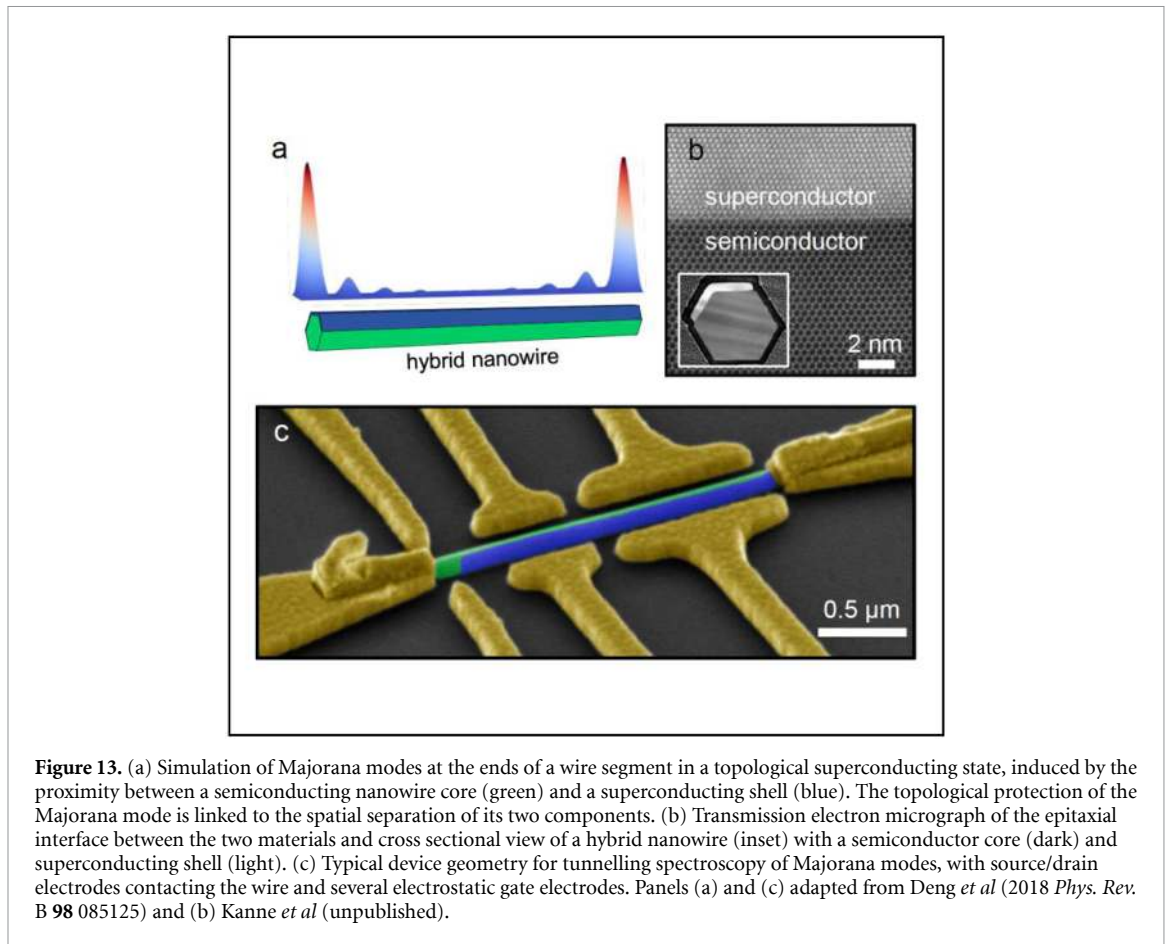


Figure 13. (a) Simulation of Majorana modes at the ends of a wire segment in a topological superconducting state, induced by the proximity between a semiconducting nanowire core (green) and a superconducting shell (blue). The topological protection of the Majorana mode is linked to the spatial separation of its two components. (b) Transmission electron micrograph of the epitaxial interface between the two materials and cross sectional view of a hybrid nanowire (inset) with a semiconductor core (dark) and superconducting shell (light). (c) Typical device geometry for tunnelling spectroscopy of Majorana modes, with source/drain electrodes contacting the wire and several electrostatic gate electrodes. Panels (a) and (c) adapted from Deng *et al* (2018 *Phys. Rev. B* 98 085125) and (b) Kanne *et al* (unpublished).

challenge in developing a scalable material platform, preferably integrated in Si-technology, which can also be coupled to other types of qubits (for universal quantum computing).

Advances in science and technology to meet challenges

Different routes have been identified towards scalable structures. The most prominent ones are based on 2DEGs [143] and selected area grown (SAG) structures [141]. These planar platforms are suited for more complex device geometries, since structures can be defined by top-down approaches using lithography, see figure 14(b). Integration in Si-technology could possibly be realized by a SAG approach, which recently has proven to be successful in growing high quality structures for optical applications. However, it is more challenging with these device geometries to control the chemical potential with bottom-gates.

As seen above several of the key challenges in observing and utilizing MZM are related to intrinsic material properties. An important direction in improving device quality is to fabricate semiconductor/superconductor interfaces *in situ* under ultra-high vacuum and at low temperatures. This results in cleaner systems with sharp interfaces [142]. *In situ* shadow structures is a powerful method to eliminate the need for etching or lift-off, as has been demonstrated for VLS based nanowire geometries and will be expanded towards SAG-based technologies [141, 144]. In addition, methods are being developed for complete *in situ* device fabrication, including normal contacts, magnetic materials, and dielectrics to realize pristine devices.

A third important development is in exploring new materials which increase the energy scale. The *in situ* growth approach allows examining a number of promising superconductors with higher critical fields [144]. In addition, TIs, such as Bi_2Te_3 and SnTe , with relatively large bandgaps are of great interest [26, 27]. Despite much effort, the challenge is still to find TIs which have an insulating bulk.

Braiding operations on MZMs would be suitable for encoding single qubit gates in quantum computing applications. Initial braiding proposals were based on physically moving Majorana modes in nanowire networks, but recent theoretical advances have led to schemes where manipulations can be obtained by adiabatic control of the interactions between MZMs or projective measurements [145]. Here both read-out and control can be performed by the same units, for instance quantum dots coupled to MZMs (see figure 14(a)). We note that only single qubit gates can potentially be realized with MZMs. Universal gates

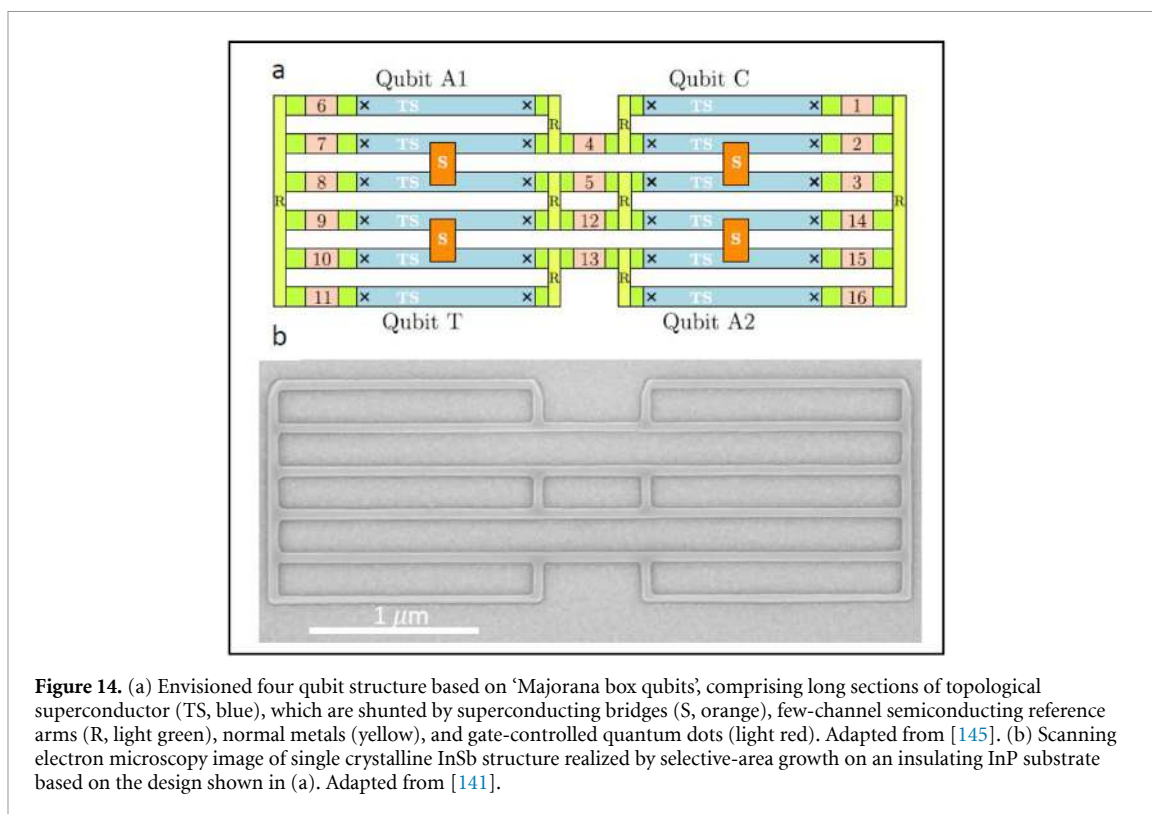


Figure 14. (a) Envisioned four qubit structure based on ‘Majorana box qubits’, comprising long sections of topological superconductor (TS, blue), which are shunted by superconducting bridges (S, orange), few-channel semiconducting reference arms (R, light green), normal metals (yellow), and gate-controlled quantum dots (light red). Adapted from [145]. (b) Scanning electron microscopy image of single crystalline InSb structure realized by selective-area growth on an insulating InP substrate based on the design shown in (a). Adapted from [141].

require that these are supplemented with other types of qubit operations. Thus topologically protected universal quantum computing is not only a matter of scaling up MZM systems.

Concluding remarks

We have reviewed concepts and materials aspects behind the advances in Majorana-based devices. During the past decade academic groups and corporate labs have jointly put significant efforts into this research. The understanding and refinement of the necessary systems has progressed and there is mounting evidence for the existence of MZMs in solid state devices. Yet, a Majorana-based qubit has not been demonstrated but it is clear that progress on topological quantum computing must go hand-in-hand with advances in materials science. We anticipate that the key topological properties of MZMs will be demonstrated the next few years. However, implementing these in complex circuits is a daunting challenge requiring heterostructures engineered with a precision at the atomic scale. Yet, these efforts have already opened up a fascinating area of science.

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10. Superconductor and semiconductor qubits

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Introduction

Quantum computation is possibly the QT with the highest transformative potential. In order to implement a quantum processor in a realistic physical platform, several requirements need to be satisfied: long qubit coherence, qubit state initialization capability, a universal set of gates with high fidelity, an efficient qubit readout, and finally, and most crucially, a scalable physical architecture.

Achieving long coherence times requires a profound understanding of the physics of the environment surrounding the qubits, particularly in the solid-state implementations discussed in this section. Eventually, qubit coherence sets a limit on gate fidelity. Incidentally, a minimum gate fidelity is required before quantum error correcting codes may be implemented to realize universal quantum computation.

Identifying a truly scalable physical platform is the most important challenge faced in the field. Implementations of just a few qubits may not show limitations appearing at larger system size. Scalability requires a truly technological boost to advance any physical platforms to become quantum processors. In recent years, the jump to this different way of operation has led to large industries take over the fundamental research developed at academic centres.

In this section, we focus on two types of solid-state architectures: superconductor- and semiconductor-based qubits. These two physical platforms are currently the most promising in realising quantum computing protocols with a solid state system. Superconducting qubits have shown robustness in scaling up the system size to the current world record 53 qubit device developed by Google [146]. Semiconductor-based qubits have also shown progress in recent years, with their true potential being the accessibility to integrate to the classical transistor technology, enabling the scalability of this platform. In addition, semiconductors can be interfaced with light to enable quantum communication to develop quantum networks.

Current and future challenges

Superconducting qubits

Superconducting materials have since their appearance represented an exciting technological opportunity. Their limited widespread use lies in the difficulty to combine the low temperatures required to operate them in real-life applications. Nevertheless, several important technologies entirely rely on superconductors, such as magnets in magnetic resonance imaging or particle accelerators. Other emerging applications may soon become a reality, such as marine cables to transfer energy generated in offshore wind turbines or faster and less energy-consuming digital supercomputers.

The non-intuitive properties of superconductors have also attracted much interest to scientists to study their fundamental quantum properties. Already in the 80s, Nobel Laureate Anthony Leggett played with the idea to control the macroscopic quantum state of a superconducting circuit exhibiting flux quantization. Late in the 90s, experiments were already at the level of exploring quantum coherent effects in devices where charge or flux quantization dominated the dynamics. Those experiments represented the birth of superconducting qubits.

The early qubits showed poor coherence properties due to their enhanced sensitivity to charge and magnetic flux fluctuations. It was not until 2004 when microwave engineering was properly introduced in superconducting quantum circuits to yield circuit quantum electrodynamics, circuit QED in short, pioneered by the Yale team [147]. This revolutionary architecture permitted separating material losses from those originating in the control and readout circuitry, as the latter were now filtered out by a resonant circuit protecting the qubit. In addition, circuit QED offered a clear path to scaling up the system size, as confirmed in successively larger devices all the way to the 53 qubit device engineered by the Google team [146]. This architecture is already being adopted by other qubit types, such as spin qubits [148].

The leading superconducting qubit types (see figure 15) [149] include the transmon qubit, consisting of a single junction shunted by a capacitor to maximize charge insensitivity, the flux qubit, a qubit sensitive to magnetic fields, and the fluxonium qubit, a single junction shunted by a super inductance, which is a precursor of topologically protected qubits, such as the $0-\pi$ qubit [150].

The quality of superconducting qubits has improved by five orders of magnitude since their inception, from nanosecond coherence times to over 100 μs [151]. At present, single-qubit gates reach fidelities better

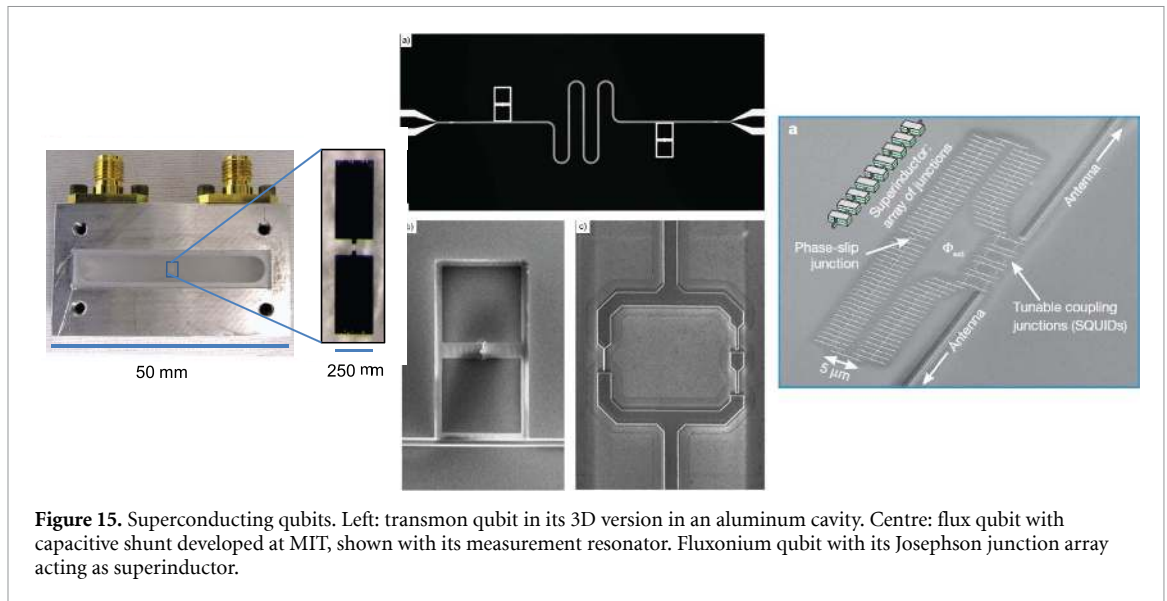


Figure 15. Superconducting qubits. Left: transmon qubit in its 3D version in an aluminum cavity. Centre: flux qubit with capacitive shunt developed at MIT, shown with its measurement resonator. Fluxonium qubit with its Josephson junction array acting as superinductor.

than 99.9%, while two-qubit gates are in the 99.8% level [146]. Despite the remarkable progress, the field faces important challenges, mostly related to material losses originated in the surfaces and interfaces of the device that limit coherence times and introduce instabilities from small but noticeable qubit parameter fluctuations. An order of magnitude improvement is required before quantum error-correcting techniques are implementable and the system can be scaled to run as a universal quantum processor. We list here the most relevant challenges:

- Qubit fabrication techniques. Since their inception, superconducting qubits have been defined with aluminum circuits. The key circuit element is the Josephson tunnel junction, usually consisting of an aluminum oxide tunnel barrier between two aluminum electrodes. The Dolan bridge technique with evaporated aluminum is the most widely used procedure, although alternative methods are being put forward, such as overlap junctions [152]. Remarkably, little has been modified in the fabrication of Josephson junctions since the early days. The amorphous nature of the junction electrodes introduces a spread in critical current values, usually in the range of 5%–10%. Reducing this number is a challenge to overcome when very large-scale systems are built and a low parameter yield is not tolerated.
- Superconducting materials. Resonators are often fabricated en-par with the same qubit material, aluminum, but often can be produced from superconductors with higher critical temperature and better intrinsic quality factors at the single-photon level such as niobium (Nb), niobium titanium nitride (NbTiN), or titanium nitride. The robustness of resonators makes them an ideal test bed for material losses that also affect qubits [153]. The use of resonators has singled out sapphire and intrinsic silicon as ideal substrates for qubit circuits. Finding superconducting materials better than aluminum is a direct path to improve qubit quality. Materials with lower microwave losses may reduce the surface contribution to decoherence. Recently [154], a team at Princeton has demonstrated qubits with record coherence times $T_1 = 362 \mu\text{s}$ and $T_{2, \text{Ramsey}} = 105 \mu\text{s}$ using tantalum and in-depth surface cleaning procedures. The insulating oxide in tantalum reduces microwave losses compared to other superconductors such as Nb. Even better materials may be soon discovered.
- Two-level defects. All experimental evidence points to the majority of noise felt by superconducting qubits originated in the surfaces and interfaces [151]. The interaction with surface losses was decreased by diluting the electric fields in large capacitors shunting the qubits [149], leading to the most significant improvement in qubit coherence in the last decade. Despite the steady increase in qubit lifetimes, the coherence times have not been enhanced significantly since 2011 when 3D cavities were introduced [155]. Another important limitation attributed to two-level defects is the observed fluctuation of the intrinsic qubit parameters, such as the qubit frequency and the qubit coherence times [156], requiring intensive calibration methods [146]. All these deficiencies are the net effect of microscopic physics with its own dynamics in close contact to the qubit states [157]. This environment turns out to be of a rather complex nature and it responds as a $1/f$ spectrum of both electric and magnetic flux fluctuations. The responsible of these fluctuations remains an area of active research, but evidence seems to point to weakly physisorbed atomic hydrogen together with free radicals originated from water-based solvents during the device production. Initial methods to mitigate their presence, such as annealing in vacuum, have been put in place [158]. Therefore, a significant amount

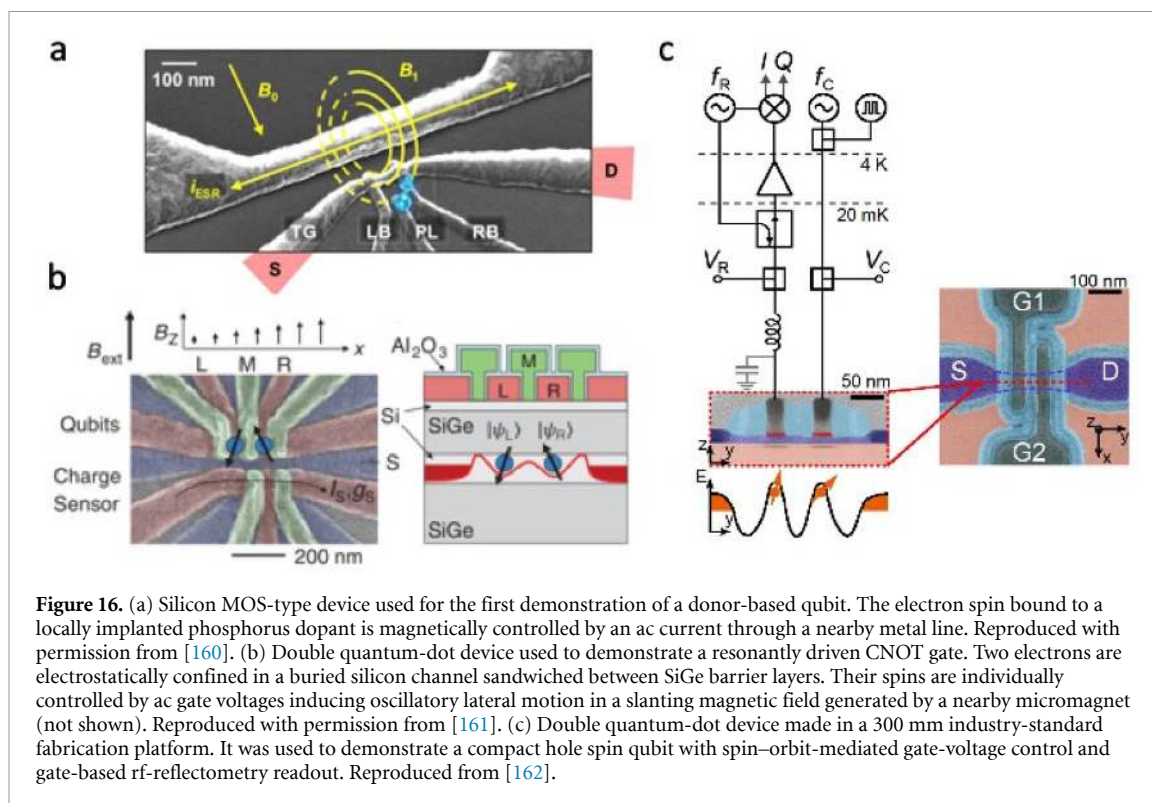


Figure 16. (a) Silicon MOS-type device used for the first demonstration of a donor-based qubit. The electron spin bound to a locally implanted phosphorus dopant is magnetically controlled by an ac current through a nearby metal line. Reproduced with permission from [160]. (b) Double quantum-dot device used to demonstrate a resonantly driven CNOT gate. Two electrons are electrostatically confined in a buried silicon channel sandwiched between SiGe barrier layers. Their spins are individually controlled by ac gate voltages inducing oscillatory lateral motion in a slanting magnetic field generated by a nearby micromagnet (not shown). Reproduced with permission from [161]. (c) Double quantum-dot device made in a 300 mm industry-standard fabrication platform. It was used to demonstrate a compact hole spin qubit with spin-orbit-mediated gate-voltage control and gate-based rf-reflectometry readout. Reproduced from [162].

of work is still required to passivate in some way the effect of the substrate noise to further enhance the qubit coherence and stabilise its parameters.

Semiconductor qubits

Semiconductors form the core materials for microelectronics and optoelectronics. The associated technologies have reached a high-level of maturity enabling large-scale manufacturing. In semiconductors, the position and motion of charge carriers (i.e. electrons or holes) can be controlled down to the single-charge level using locally applied electric fields. This possibility has enabled the realization of quantum devices in which carriers are confined to form low-dimensional systems with quantized energy levels. In particular, quantum dots are zero-dimensional objects where carriers are confined in all spatial directions resulting in a discrete energy spectrum (typical level spacing of 0.1–10 meV, depending on material and size). Due to the local Coulomb repulsion, charge occupation in quantum dots is also quantized, provided temperature is lowered below the characteristic charging energy (typically 1–10 meV). Following technical advances in the last couple of decades, it is now routinely possible to obtain quantum dots confining only one electron or one hole.

The spin degree of freedom of a single particle in a magnetic field provides a natural two-level system to encode an elementary bit of quantum information. This idea lies behind the seminal proposal of Loss and DiVincenzo who envisioned a quantum-computing device based on electron spins in quantum-dot arrays. Around 20 years ago, this proposal triggered a world-wide experimental endeavour focusing initially on few-electron quantum dots made in GaAs-based heterostructures. (See [159] for a review on the early age of semiconductor spin qubits). The first spin qubits were reported in 2005. Soon, however, scientists realized that the unavoidable hyperfine interaction with the nuclear spins of the host crystal causes a rapid dephasing of the electron spin state on a time scales of only tens of nanoseconds.

This serious problem can be avoided by turning to semiconductor materials with zero nuclear spin. That is the case of group-IV semiconductors (e.g. C, Si, and Ge) whose most abundant isotopes are nuclear-spin free.

Presently, research is mostly focusing on silicon, mainly because of its well-established technology. In addition, silicon offers a range of opportunities for storing and controlling quantum information. Soon after Loss and DiVincenzo, Kane proposed the realization of spin qubits encoded in the nuclear spin of phosphorous dopants properly implanted in a silicon device.

The first silicon qubits were reported in 2012 (see figure 16(a)). A few years later, the advent of the first devices made from isotopically purified silicon was a turning point, leading to the development of electron-spin qubits with much longer coherence times. To date, the best silicon qubits have surpassed the

threshold for quantum error correction, scoring single-qubit fidelities above 99.9% [163, 164]. The implementation of two-qubit gates is still at an early stage with only a few reported demonstrations (see e.g. figure 16(b)) [161, 165–167]. While a two-qubit fidelity of 98% has been reached so far, ways to go well beyond have been identified [166].

Following this remarkable progress, silicon-based qubits have become serious contenders for the development of quantum processors. Their potential relies on the possibility of leveraging the large-scale integration capabilities of silicon technology. In this prospect, efforts have begun to focus on the implementation of qubit functionalities in devices made in industry-standard fabrication platforms (see e.g. figure 16(c)) [162].

Different architectural schemes have been recently proposed to face the scalability challenge. These schemes involve strategic choices based on the current state-of-the-art. Given the multifaceted nature of semiconductor spin qubits, which is far from being thoroughly explored, an evolution of these initial ideas can be expected in compliance with the forthcoming progress. At the level of physical system, control toolbox, and material, a variety of alternative options are currently being benchmarked against each other in order to identify the most promising one with respect to scale-up. We list some of the most relevant ones:

- *Electron- vs hole-spin qubits*: electron quantum dots exhibit lower-disorder and lower variability. Electron spin qubits have longer coherence times and have shown both one- and two-qubit functionality with the highest fidelities. Hole spin qubits do not suffer from the valley degeneracy problem. Hole spins enable all-electric fast control (see [162, 168]).
- *Dopants vs quantum dots*: Dopants allow for longer coherence times [160]. Their atomically-precise positioning, either via local implantation or scanning probe lithography is challenging, while quantum dots are deterministically defined by gate voltages. Quantum dots show so far a clear advantage with respect to implementing inter-qubit coupling and creating multi-qubit arrays.
- *Single-electron vs multi-electron qubits*: Encoding a qubit onto multi-electron electron spin states (e.g. singlet and triplet states) is a way to enable electric-field controlled qubit rotations [169]. This, however, has a price in terms of device complexity making scalability more cumbersome with respect to the Loss-DiVincenzo spin-1/2 encoding.
- *Electric dipole spin resonance*: exploits either intrinsic [162] or synthetic [163] SOC. While it allows for faster all-electrical spin manipulation, the spin qubit becomes sensitive to charge noise, which degrades its coherence. Magnetic-field-drive electron spin resonance applies well in the absence of SOC but qubit manipulation times are typically longer.
- *Si MOS vs SiGe heterostructures*: quantum dot qubits defined in a Si MOS structure are more readily compatible with main-stream CMOS technologies. In addition, the stronger electric fields in MOS structures favor the lifting on valley degeneracy. Quantum dots defined in a buried SiGe/Si/SiGe strained QW show a lower level of disorder. Recently, SiGe/Ge/SiGe confining high-mobility holes are also emerging as a promising alternative system combining low disorder and electric-field spin control [168].

Transverse research developments

The stringent requirements to scale up the size of any quantum system unavoidably leads to novel enabling classical and QTs that may be suited to several physical implementations. In particular, there already exist transverse, enabling classical and QTs developed for superconducting qubits that can be applied to semiconductor qubits. We list some of the most interesting ones here:

- (a) **Josephson parametric amplifiers for fast high-fidelity spin readout.** The development of both narrow and, especially, wide band near quantum-limited superconducting parametric amplifiers [170] to simultaneously readout multiple qubits is a necessary step in ramping up the complexity of devices. This technology can be applied to any solid-state quantum computing platform and its operation can extend to sub-GHz frequencies, which is interesting for semiconductor qubits [171].
- (b) **High impedance circuits.** High-impedance resonators based on Nb, NbN, NbTiN, and arrays of superconducting quantum interference devices have been employed for fast single-shot spin readout and for the coherent coupling of distant spin qubits [172]. In parallel, an old superconducting material known as granular aluminum has been introduced in superconducting qubit technology in recent years [173]. This material is obtained by leaking a small amount of clean oxygen during the deposition of aluminum. The resulting thin film contains microscopic aluminum grains embedded in an aluminum oxide matrix. The aluminum grains are connected to each other by Josephson tunneling, resulting in a meta-material that behaves as a continuous medium at GHz frequency. The material is endowed with genuine properties which find applications in QTs with superconducting circuits: high kinetic inductance, low-level losses and high critical magnetic field, on the order of several Tesla. The most important is the high kinetic

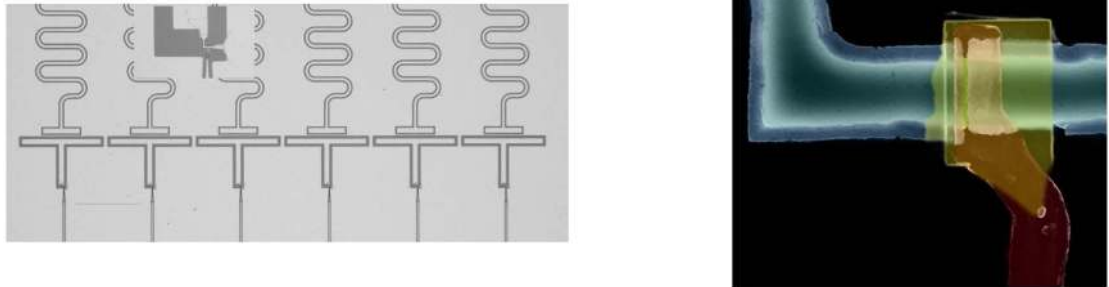


Figure 17. Gatemon qubit. Left: gatemon array. Right: closeup of the gatemon junction with an electrode to tune the static potential and change the tunnel barrier electrically. Reproduced with permission from [176].

inductance per square, ranging up to several nH/square, which combined with low losses result in a true superinductor with impedances well above the resistance quantum, $R_Q = h/(2e)^2 \approx 6.5\text{k}\Omega$. This material is analogous to superinductors obtained by large area Josephson junction arrays used in wide-band parametric amplifiers and fluxonium qubits. In fact, a high-coherence fluxonium obtained with granular aluminum has already been demonstrated. Although intrinsically small, the nonlinearity of the material itself can be engineered large enough to be an alternative to Josephson junctions, as already demonstrated in a transmon-like qubit combining aluminum and granular aluminum. This material may play a relevant role in exploring light-matter interactions in the ultrastrong coupling regime [174].

- (c) **Classical control cryogenic technology.** Superconducting digital circuits have been known for many decades. Based on single flux quantum ideas, classical transistor-based logic can be implemented, providing very fast and very low power electronics. This kind of technology is advancing to become an essential component in any solid-state quantum computing platform, already extensively used by the company D-Wave producing quantum annealers with over 2000 qubits [175].

Conversely, some semiconductor-based developments may be beneficial to superconducting qubits. We list here two examples:

- (a) **Hybrid superconductor-semiconductor qubit: Gatemon.** Groups in Copenhagen [176] and Delft [177] have developed a superconducting transmon qubit, the so-called gatemon, whose transition frequency can be tuned by a gate voltage (see figure 17). This type of qubit incorporates a Josephson junction consisting of an InAs semiconductor channel with superconducting Al contacts grown *in-situ*. The Josephson energy, directly linked to the qubit frequency, depends on the carrier density in the semiconductor channel, which is gate dependent. Gatemon coherence times of about $10\ \mu\text{s}$ have been reported, as well as single- and two-qubit gate operations. In contrast to flux-tuned transmons, voltage-tunable gatemons may offer a valuable path to large-scale qubit integration.
- (b) **Cryo-CMOS.** Classical cryogenic electronics based on silicon CMOS technology is a natural choice for semiconductor-based qubits. Since recently, cryo-CMOS is being applied also to superconducting quantum hardware. For instance, the Google team recently developed a first prototype of quantum-control circuit based on 28 nm CMOS technology [178]. The circuit was mounted on the 3 K stage of a dilution refrigerator to perform XY gate operations on a small set of transmon qubits at base temperature.

Concluding remarks

The most dramatic improvements in superconducting qubit technology to produce working qubits have come from both the circuit design surrounding the qubit, as well as the quality of the materials of the circuit, the substrate, and the interface between them. The challenge of obtaining a stable enough superconducting qubit has to be faced principally from a more profound understanding of the microscopic processes occurring in the neighbourhood of the qubit. Finally, the challenge of further increasing the system size will put even more stringent demands on technological advancements, both classical and quantum mechanical.

Progress toward a semiconductor-based quantum processor will hinge upon finding the best compromise in terms of high one- and two-qubit fidelities, low variability, and scalability of the qubit design. Extending the coherence time and the fidelity of qubit operations will require a tremendous engineering effort at the level of materials (optimization of gate stacks, material interfaces, isotope engineering, dopant incorporation, etc) and device design (maximal control fields, minimized effect of charge noise, etc). Increasing the number

of qubits will necessarily involve the development of ad-hoc control/readout hardware. As envisioned in the aforementioned proposals [179, 180], elements of this hardware may lie close to the qubits. In this prospect, the development of cryogenic CMOS electronics sharing the same silicon technology is particularly appealing since it would allow for a certain level of quantum–classical co-integration [181].

Eventually, a combination of the technological advances in superconductor- and semiconductor-based qubits may be the path to a hybrid solid state universal quantum computer.

Acknowledgments

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11. Non-equilibrium phenomena in quantum materials

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Status

Much of our technology relies on the non-equilibrium control of solids, from dynamically switching transistors in logic circuits, to reading and writing memory devices, to various energy harvesting applications [182]. This has bred interest in exploring solid-state phenomena that are inherently non-equilibrium, with an eye on creating functionalities that can be manipulated efficiently and at high speeds. Advances harnessing light–matter interaction using ultrafast laser pulses are shifting materials research in this direction, where remarkable quantum effects have been discovered that are already leading to device applications.

A notable early success was the sub-picosecond demagnetization of a ferromagnetic metal [183]. Multiple ultrafast thermal and non-thermal pathways to optically control magnetism have since been discovered [184], and these effects are now being used in next-generation magnetic storage devices [185].

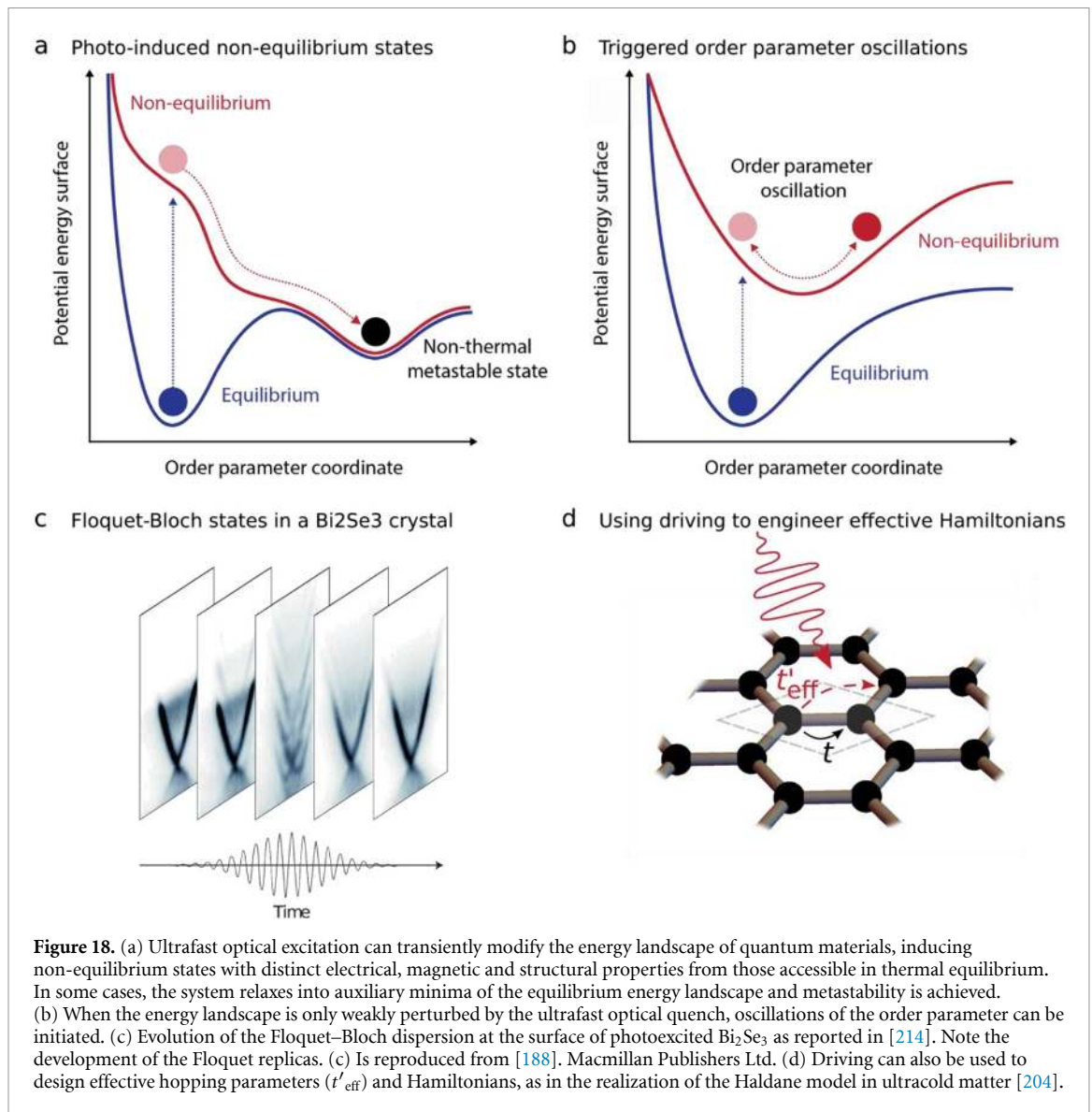
More exotic phenomena can be found in complex solids. In these systems, optical excitation can shift the delicate balance between coexisting or competing ground states, inducing non-equilibrium states with distinct electrical, magnetic and structural properties from their equilibrium counterparts (figure 18(a)) [186–188]. In most cases, these states are transient and decay on the order of femtoseconds to nanoseconds. However, in some cases, persistent metastable phases are obtained that survive indefinitely on experimental timescales [189–191]. 1T-TaS₂ is an interesting example, where the insulating ground state and a metallic metastable state can be independently triggered-and-held by using different colour laser pulses [191]. This unusual functionality is now being considered as a memory device in future low-temperature electronics.

In recent years, advances in laser technology have enabled the selective excitation of collective modes in quantum materials. Resonantly driven phonon modes, for example, can induce directed lattice distortions that have served as a control knob for ferroelectricity [192, 193], magnetism [194] and insulator-to-metal transitions [195]. But perhaps the most striking example is light-induced superconductivity [196], where the optical signatures of superconductivity have been observed in materials well above their equilibrium transition temperatures. This phenomenon has been observed in multiple cuprate and organic superconducting compounds [196–198], suggesting that it may be a common effect associated with strongly correlated superconductivity.

The non-equilibrium dynamics induced by ultrafast optical stimulation can also reveal important information about the ground state of quantum materials, such as the presence of coexisting phases, electron-boson coupling strengths, and the magnitude of correlation-induced energy gaps [199, 200]. Pulsed excitation can even initiate oscillations of a phase's order parameter (figure 18(b)), as has been observed in CDW systems [199–201], superconductors [202] and excitonic insulators [203]. This phenomenon provides a novel way to map the free energy landscape of solids, and with further research could serve as a reliable probe of order parameter symmetry.

Much of the research to date has focused on the non-equilibrium effects induced in solids immediately following impulsive photo-excitation. In more recent years, the ability to generate strong-field optical pulses at longer wavelengths—where light–matter interaction is inherently enhanced—has led to a surge of interest in exploring phenomena that occur *during* optical illumination. Experiments are now in the regime where the material response is governed by the coherent dressing of its quantum states by the light field. Such processes can be described using Floquet theory [205, 206], a non-perturbative and non-adiabatic framework that enables time-periodic Hamiltonians to be mapped to an effective static Hamiltonian. This mapping enables the highly developed theoretical infrastructure used to describe equilibrium solid-state physics to be applied to the non-equilibrium regime, which has led to some exciting predictions that are just starting to be tested.

One of the cornerstones of 'Floquet-engineering' in solids was the prediction of laser-induced band gaps in graphene [207, 208], which was signalled to have an experimental sweet spot in the mid-infrared [209]. Since 2013, unique time-resolved ARPES experiments [210] demonstrated two crucial points. First, the appearance of Floquet–Bloch states—the photon-dressed electronic states in a crystal—through the visualization of a seemingly abstract band structure (figure 18(c)). Second, the opening of polarization-dependent band gaps in the dressed band structure. Beyond these spectral modifications, it was also predicted that Floquet–Bloch states can be topologically non-trivial [208, 211, 212] (for a review see [206]), which in Dirac systems requires breaking TRS through circularly polarized light [211]. These ideas were initially tested in photonic [213] and cold atom [204] (figure 18(d)) experiments simulating graphene, but it was not until



very recently that one of the most celebrated consequences of topological Floquet-engineering—the light-induced anomalous Hall effect [208, 211, 215]—was demonstrated in condensed matter [216].

Current and future challenges

The overarching goals of this field are twofold. First, to understand the physics of solids away from thermal equilibrium, where quantum effects that have no equilibrium counterpart can be realized. Second, to use this knowledge to design functionalities that will have real technological impact.

This is a relatively young field and research to date has largely been that of exploration. In order for the field to mature, it is necessary to move beyond surveying the types of effects that can be induced and focus on understanding the overarching concepts that unify many of the phenomena already discovered.

Some important challenges include, but are not limited to:

- Devising materials and driving protocols for the realistic implementation of Floquet-engineering proposals in the face of dissipation, bath coupling and electronic heating [217, 218]
- Improving our understanding of old problems such as shift photocurrents, though with much applied interest still lack a unified framework (see [219] and references therein)
- Improving our understanding of space-time symmetries to control driven disordered systems, either to achieve unprecedented topological phases [220], or new concepts such as time-crystals [221]
- Developing a coherent framework for dealing with new non-equilibrium topological phases including Floquet and non-Hermitian systems [222]
- Understanding the mechanisms behind photo-induced phase transitions and metastability

- Mapping non-equilibrium order parameter symmetries
- Improving our understanding of how directed lattice excitation can create new non-equilibrium phases of matter
- Turning non-equilibrium phenomena into functionalities by experimenting with devices
- Designing materials that host desirable non-equilibrium effects at higher temperatures for future applications

One path to addressing the challenges listed above is to increase feedback between experimental characterization, theoretical understanding, and materials synthesis—a successful strategy employed in many other branches of quantum materials research [182]. Experiments have long been the driving force in this field, and our theoretical understanding is steadily improving. But at the moment there is little emphasis on developing materials or heterostructures that are designed to host a given non-equilibrium phenomena when photo-excited. Doing so would allow researchers to more systematically test non-equilibrium theories and ultimately create new functionalities. Let this be a call for an era of intentional non-equilibrium materials design.

Advances in science and technology to meet challenges

Experimentalists are now well-equipped with ultrafast light sources spanning the THz to the hard x-ray regime and a wide range of available spectroscopic probes. Many spectroscopies still suffer from poor signal-to-noise, but this will naturally alleviate as laser pulse train repetition rates continue to increase. There is also a need for ultrafast electrical and scanning probes, which are currently being developed [216, 223, 224]. Conceptually, the biggest experimental leap will occur once non-equilibrium phenomena can be engineered using cavities instead of strong laser pulses. This exciting research front is only just getting started [225–227].

On the theoretical side, the field will greatly benefit from the use of quantum simulators, as well as recent advances in time-dependent density functional theory (DFT) allowing for a linear scaling with system size [228]. New learning algorithms built on these new state-of-the-art methods could also completely reshape our present simulation capabilities.

Concluding remarks

Here we have given a brief overview of how coherent light–matter interaction can induce a wide range of non-equilibrium phenomena in quantum materials that could serve as functionalities in next-generation technologies. Distinctly motivated research fronts are intertwining and synergizing with other fast evolving topics such as topological phases of matter. We expect that recent technological advances, together with increased feedback between experiment- and theory-driven perspectives, will bring surprises in the coming years. Indeed, catalyzed by recent discoveries, the physics of non-equilibrium phenomena in quantum materials is becoming an even more promising *terra incognita*.

Acknowledgments

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12. 2D hyperbolic materials

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Status

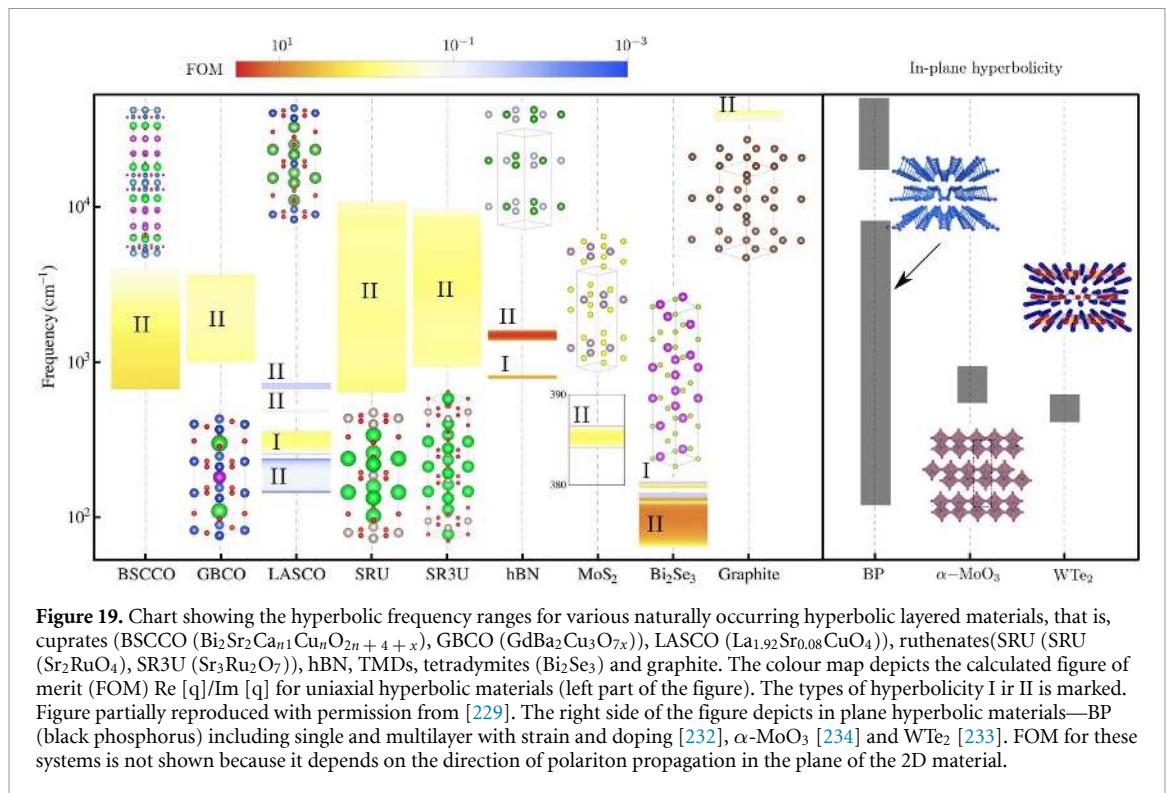
Hyperbolic materials (HMs) are systems where their optical permittivity tensor components have opposite signs. These materials can accommodate polaritonic modes due to dipole excitations of various origins, such as plasmons and phonons [229]. The constant energy surface ($\omega(\mathbf{k}) = \omega_0$) for the polariton modes in such a material takes the form of a hyperboloid (or hyperbola in 2D) in wavevector space. In contrast, most common materials have an ellipsoidal isofrequency surface for their supported polaritons. The unique hyperbolic topology of the k -space in these materials provides access to unprecedentedly large optical density of states, fundamentally changing the nature of light–matter interaction. This property leads to a number of technologically relevant applications in the field of subwavelength imaging, biosensing, modulators, high precision internal structure diagnosis, thermal emission control and spontaneous emission enhancement ([229] and references therein). Traditional realizations of such HMs so far have been through artificially structured media called metamaterials or metasurfaces, where a carefully chosen geometry of constituent unit cell leads to an ‘effective’ permittivity tensor which is hyperbolic. Apart from the constraints of nanofabrication, this approach has a fundamental limitation since the inverse of the unit cell size limits the maximum wavevector for the polariton.

The past several years have seen the emergence of a new class of naturally occurring 2D vdW HMs, covering a hyperbolicity range from the visible all the way up to the mid IR wavelength range [229]. The hyperbolic behaviour in these materials covers a range of collective excitations—plasmons, phonon polaritons and excitons, which not only opens up avenues for novel applications but also for exploring the fundamental nature of these polaritons in the presence of hyperbolicity. The first experimental report of natural 2D HMs appeared in 2014, where the hyperbolic modes were observed via scanning near field optical microscope [230], followed by a number of other demonstrations, including far-field scattering measurements of HM nanostructures [231]. Multilayer hexagonal boron nitride (hBN) was shown to have a negative in-plane permittivity in the frequency range 1360–1610 cm^{-1} and a negative out of plane permittivity in the range 760–825 cm^{-1} . Subsequent to this work, several 2D HM candidates were identified including black phosphorus [232], TMDCs [233], transition metal oxides such as α - MoO_3 [234], cuprates, tetradymites and graphite [229]. In figure 19, we present a library of these layered 2D HMs, where the spectral range and type of the hyperbolicity as well as the losses of the hyperbolic polariton mode quantified by a figure of merit FOM given by the ratio of the propagation length ($1/\Im k$) to the approximate polariton wavelength ($\sim 1/\Re k$) for the allowed wavevector k is presented [229]. Among these, a particularly interesting class of 2D HMs are ones that show natural in plane hyperbolicity such as MoO_3 and WTe_2 [233] and black phosphorus [232].

There have been several efforts at experimentally detecting the hyperbolic nature of the polaritons in these materials, the most straightforward being through near field scanning microscopy [230] and photo induced force microscopy [235]. In both cases, the hyperbolic polariton is launched by a nanoscale tip close to a 2D HM structure, however the former detects the light intensity whereas the latter measures the optomechanical force at the tip. The measured interference patterns reveals the wavevector at different excitation frequencies. Far field scattering measurements have also been used to detect hyperbolicity in the nanostructure of these 2D HMs, where the polarization and incidence angle dependences of the obtained scattering cross sections from these 2D HMs highlights the hyperbolic response [231].

Future and current challenges

2D HMs are interesting for future applications, but several challenges remain outstanding. A critical constraint is the wafer scale growth of the 2D HMs [236]—most experimental demonstrations so far have employed mechanically exfoliated films with typical flake size on the order of tens to hundreds of microns only. Moreover, this method does not offer precise control on the number of layers of the 2D HMs. Hence, any macroscale application of 2D HMs is currently prohibitive as wafer scale platform would require uniformity in crystal orientation and layer numbers. There have been several efforts in the direction of large area growth of these systems, but large scale manufacturing of 2D HMs is still in its infancy [237]. As highlighted in figure 19, another fundamental challenge with these 2D HMs is the large Ohmic losses, particularly in the 2D HMs which rely on plasmons. This is a fundamental limitation related to intraband damping and the losses associated with interband transitions in these materials [238]. For applications that



rely on spontaneous emission enhancement near 2D HMs, these losses lead to the phenomenon of quenching of the emission. Moreover, the propagation lengths of the hyperbolic polaritons become prohibitively small for any waveguiding applications [238]. A third challenge is the environmental stability of these 2D HMs [239]. For instance, black phosphorus has been shown to be unstable in ambient atmosphere which leads to deterioration in its optical response. Similarly it has been shown that upon room-temperature exposure to the environment for several months, TMDCs show aging effects such as cracking, changes in morphology and deteriorated optical response ([239] and references therein). The fourth challenge is the active tunability of the hyperbolic modes [240]. 2D HMs, particularly those in the mid-IR range, rely on phonon polaritons whose spectral region is fixed by the longitudinal and transverse optical phonon frequencies. This is a disadvantage in terms of the spectral coverage as well as the fixed dispersion of the phonon polaritons within the Reststrahlen bands.

Advances in science and technology to meet challenges

To meet the first challenge, namely large area growth, several recipes have been formulated [236]. Firstly, there have been improvements in the mechanical exfoliation itself, for instance using a gold film, introducing additional plasma and heat treatment steps. Particularly, for TMDCs, metalorganic chemical vapour deposition has resulted in wafer scale growth [241]. For hBN, wafer scale growth has recently been demonstrated with precursors fed into molten gold and copper thin films [241]. For wafer scale $\alpha\text{-MoO}_3$, a plasma enhanced chemical vapour deposition technique has been demonstrated [242]. For black phosphorus, an approach involving the conversion of red phosphorus to black phosphorus demonstrated a millimetre scale growth [243]. Despite these promises, these methods need further development for compatibility with substrates of technological interest.

Regarding overcoming the optical losses in 2D HMs, incorporation of optical gain has been used [244], as was theoretically considered in [232] for black phosphorus. For hBN, the quality factor can be improved with isotopically enriched samples, which typically have narrower linewidths than mixtures of isotopes [245]. Another approach is working in a frequency regime where interband losses do not dominate. Here the spectral tunability of this low loss regime could be obtained by making heterostructures of 2DMs [238]. Experimental reports on both these fronts have so far been limited. The problem of instability of 2D HMs has been most severe for TMDCs and black phosphorus. Typical methods of improving on this front involve thermal treatment and encapsulation layers. Among the latter, deposition of thin protective oxide layers via atomic layer deposition have shown promise. For black phosphorus in particular, hBN encapsulation has also shown promise. A low cost encapsulation technique based on organic coatings such as PMMA and PTCDA has been demonstrated. However, in the long term, such organic coatings fail to completely protect the 2D

HMs from oxygen and water. As an alternative, certain chemical modification techniques are also being explored which protect the 2D HMs by covalent bonding to the surface [239].

Lastly, the tunability of phonon polariton based 2D HMs is an active area of research. One possibility is the use of carrier photoinjection which has been demonstrated in other systems such as InO and 4H-SiC [246]. Tunability of hyperbolicity in black phosphorus using electrostatic gating, strain and optical pumping has been theoretically predicted [232]. There is also a recent interest in manipulating the polaritons of 2D HMs by integrating them with phase change materials such as VO₂ as well as other 2D plasmonic materials such as graphene, whose plasmons can be tuned electrostatically. For the emerging field of in-plane hyperbolic materials, recently the polariton dispersion manipulation has been experimentally demonstrated via topological transitions induced via twisting of two α -MoO₃ layers [247]. The possibility of active tunability of the hyperbolic polaritons and the extension of this active tunability to other 2D HMs and heterostructures presents enticing opportunities [245].

Concluding remarks

The field of 2D HMs presents several exciting open questions both from the point of view novel materials as well as improving the stability and active tunability of existing systems. Although the field is its infancy, it is rapidly growing and shows promise for many emerging applications.

Acknowledgment

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13. Spin torque materials

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Status

In the late 90's it was discovered that a spin-polarized current can be used to manipulate the magnetization of a ferromagnet. This raised the interest not only of the spintronics community, but also of technological companies [248]. The new effect could be used in magnetic random-access memories (MRAMs), which store information in the magnetization orientation of nanoscale magnetic elements (figure 20(a)). The concept is simple: a charge current is converted into a spin current (or a non-equilibrium spin density), which in turn creates a torque on the magnetization (called 'spin torque') that can switch the magnetization orientation. This approach helped overcome the scaling limitations posed by the available MRAM technology at the time, which relied on external magnetic fields.

The charge-to-spin (CS) conversion can be achieved by different strategies. In the first generation of commercialized spin-torque MRAMs, so-called spin-transfer torque (STT) MRAM, a ferromagnetic layer is used as a polarizer in a vertical magnetic-tunnel junction (MTJ) structure (figure 20(b)) [248]. However, large current densities across the junction are required to switch the magnetization, resulting in reliability issues. A route to circumvent this problem relies on exploiting materials with large SOC in contact with the magnetic element. In this case, the electrical current flows along the film stack, instead of across it, enhancing the device endurance. The CS-conversion process may involve bulk and interfacial SOC mechanisms (including, but not limited to, the SHE and the Rashba-Edelstein effect), opening the path for the next generation SOTs MRAMs [249, 250].

Magnetic memories based on spin torques are non-volatile, and offer low power consumption, high endurance, high speed, good packing density and scalability. These include memories based on the above-mentioned STT or SOT (in an MTJ structure), as well as other types of memories based on domain wall motion such as the 'race-track memory', a solid-state alternative to hard-disk drives due to its potential for 3D high-density integration and no moving components.

STT-MRAMs have reached technological maturity (focusing mostly on CoFeB/MgO-based MTJs) and their major challenges are expected to be mostly about material engineering, rather than fundamental discovery of novel materials (except maybe using vdW heterostructures). The following discussion is therefore focused on the promising alternative of SOT-MRAM, which is still in the accelerated research phase.

SOTs promise better efficiency and speed than STTs, and enable the switching of antiferromagnets and magnetic insulators as well as the generation of coherent spin waves [249]. However, it remains a central scientific challenge to tune and engineer more efficient heterostructures. A common figure of merit and a full comprehension of the SOT phenomena in most systems are still lacking, hindering a straightforward comparison between the reported spin-torque efficiencies in different studies [249]. In parallel, new 'spin torque' materials and pathways are being considered to meet the demands of increased efficiency, downscaling and switching without external magnetic fields at ultrafast speeds (figure 21).

Current and future challenges

One major challenge is the need to reduce the current density required for magnetization manipulation and, with it, the power dissipation in devices. Using heavy metals (Pt, W) as large SOC-materials has so far rendered a CS conversion significantly below 100% [250]. To overcome this limitation new types of materials are being investigated, including TIs, for instance Bi₂Se₃ or (Bi_{1-x}Sb_x)₂Te₃ (figure 21(a)). TIs are insulating in the bulk but possess conducting, topologically-protected surface states in which the spin polarization is determined by the carrier propagating direction. The CS conversion efficiency of such TSS is potentially larger than those in Rashba split states. In fact, large SOT in TIs has been reported [252, 253], while magnetization switching has already been achieved. The SOT efficiency is highly dependent on interfacial properties [254] but it has been claimed to be more than one order of magnitude larger than that obtained with heavy metals.

Parallel efforts are being made towards miniaturization of devices in which 2DMs can play an important role as we strive for ultrathin and flexible electronics (figure 21(b)). TMDCs, which include some Weyl and Dirac semimetals, are gathering increasing attention as their spin textures could give rise to large CS conversion [255, 256]. Furthermore, the recent discovery of 2D ferromagnetic materials with metallic, e.g. Fe₃GeTe₂, or insulating, e.g. CrI₃, behaviour, open respectively the possibility of replacing the thick metal layers in conventional MTJs or creating new spin-filter MTJs that use spin-polarized tunnel barriers [257].

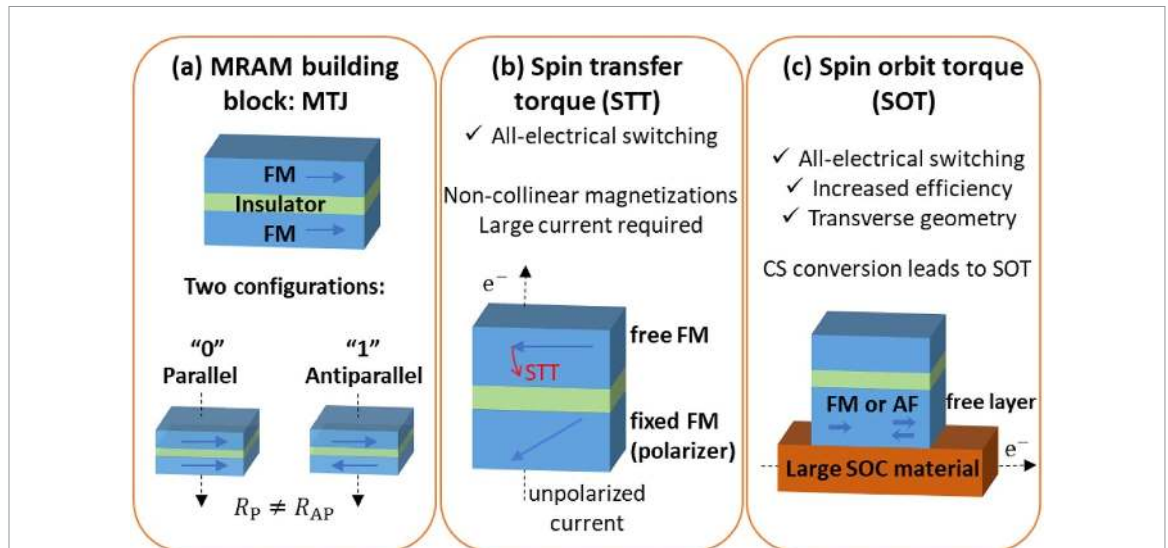


Figure 20. (a) Magnetic tunnel junctions are the building block of MRAM: the (parallel or antiparallel) orientation of the magnetization of two ferromagnets sandwiching a thin insulating layer defines two different states of resistance; (b) a fixed ferromagnet polarizes the current, and large (polarized) current allows the switching of the free ferromagnet by STT; (c) current flow along a material with large SOC generates a torque on an adjacent magnetic layer (ferromagnetic or antiferromagnetic), allowing its manipulation. Note that it is also possible to achieve magnetization switching by SOT in a magnetic material with large SOC, effectively combining the functionality of the two layers in one.

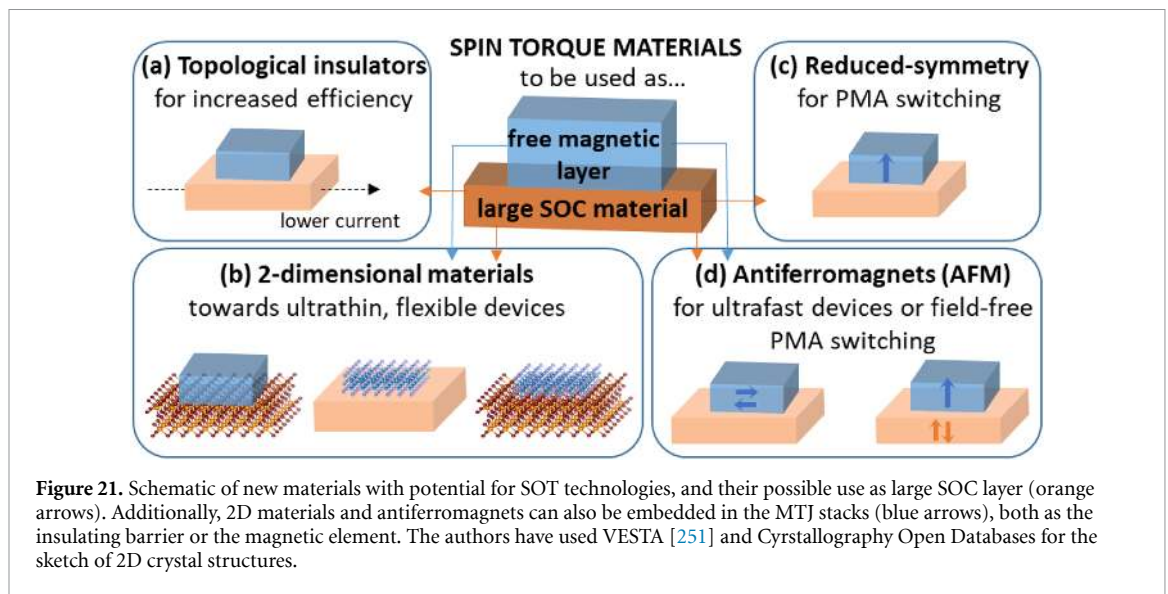


Figure 21. Schematic of new materials with potential for SOT technologies, and their possible use as large SOC layer (orange arrows). Additionally, 2D materials and antiferromagnets can also be embedded in the MTJ stacks (blue arrows), both as the insulating barrier or the magnetic element. The authors have used VESTA [251] and Crystallography Open Databases for the sketch of 2D crystal structures.

The reduced thickness of the overall structure with 2DMs could help overcome current limitations regarding fabrication and planarization, which are affecting the scaling of current complex MTJ pillars whose overall thickness exceeds tens of nanometres. At the same time, implementing tunnel barriers with 2DMs, such as hBN or graphene, which are atomically thin and smooth, would solve tunnel barrier uniformity and material intermixing issues that are arising with bulk insulators such as MgO in the ultrathin limit [258].

Another non-trivial matter is the all-electrical switching of magnetic elements with perpendicular magnetic anisotropy (PMA), which are favoured due to their better scalability for MRAM implementation (figure 21(c)). This requires torques of a certain symmetry [259], not achievable in most heterostructures (for example with heavy metals), so that switching may only be accomplished with the help of an external magnetic field. Recent reports, however, have shown that taking advantage of the reduced symmetry of the 2D semimetal WTe_2 or β - $MoTe_2$, torques with this type of symmetry can be obtained [255, 256]. Alternative strategies including wedged structural engineering, the use of ferroelectric substrates, domain wall pinning by geometry engineering or even taking advantage of exchange coupling, have also been considered [250].

Increasing the operation speed further motivates the study of SOT in antiferromagnetic materials [249, 260]. These are especially suited for ultrafast devices because their magnetization dynamics, governed by exchange fields, is in the THz range (whilst in ferromagnets it is limited to GHz). Antiferromagnets are

being studied both as the SOT source and as the magnetic layer to be manipulated (figure 21(d)). Additionally, the lack of a macroscopic magnetic moment could help increase the integration density in magnetic memories, as well as field-free switching of PMA nano-objects by taking advantage of exchange coupling between a ferromagnet and an antiferromagnet.

Advances in science and technology to meet challenges

The study of SOTs is a young research field and new types of spin torque materials are still flourishing, which accounts for the relatively few antiferromagnets, TIs or 2DMs that have been so far investigated. It is thus expected that many new results with novel materials will arise in the near future. Considerable progress is being made in material science towards developing high-quality heterostructures but further advances are required. They include achieving material growth optimization and large-scale integration of, for example, TIs, Weyl and Dirac semimetals and 2DMs with controlled thickness [259], as well as improving interfacial quality within the heterostructures' layers. Impurities (source of extrinsic contributions to the SOC), crystalline symmetries, interface oxidation and intermixing greatly influence the observed spin properties [249, 250, 254]. Therefore, a better control of such parameters will help us advance in the reproducibility and engineering of the torques, while facilitating the understanding of the underlying physical mechanisms. Moreover, in view to consider the use of such devices in industry, further research on the compatibility of the new materials with the current Si-based technology is still pending [259].

Progress in the understanding of microscopic torque mechanisms requires the identification of the origin of large discrepancies between the reported SOT efficiencies with similar systems, which are characterized at different laboratories or with different methods [249, 253]. The wide variety of effects unrelated to SOTs that contribute to the detected signals, from Oersted fields to thermoelectric effects, illustrates the need for comparing the results obtained with alternative experimental techniques using the same heterostructure. The complex nature of the phenomena must be taken into account in the experimental design, motivating systematic measurements as a function of temperature, thickness or interlayers [249] and calling for complementary experiments with advanced characterization methods.

Concluding remarks

SOTs represent a unique opportunity to electrically manipulate magnetic layers, enabling increased efficiency and speed towards devices such as the SOT-MRAMs exemplified above. Despite the necessary progress required both for their understanding and optimization, the potential of SOTs for applications goes well beyond simple increased MRAM performance, as it can provide novel functionalities within other technologies, for instance memristors and nanooscillators for neuromorphic computing [261].

There exists a wide variety of materials with potential in spin torque structures (for example within the families of 2DMs or TIs), each with distinct and unique properties. These materials are being thoroughly studied in other areas of condensed matter physics, offering a rich playground for interaction between fields, with much scope for yet unimaginable new applications.

Acknowledgments

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14. Magnetic skyrmions

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Status

Alike Majorana fermions, the concept of skyrmions originates from elementary particle physics and has inspired physicists to explain various quantum phenomena such as the quantum Hall effects. Over the past years magnetic skyrmions have become a major area of interest within the field of spintronics due to its novel physics, stimulated by the vibrant interest on topological states of matter, and its great potential for applications.

Magnetic skyrmions [262, 263], bridging topology and magnetism, are local excitations in a homogeneous magnetic domain state with unique real-space topological characteristics [264]. They are part of a broader family of chiral magnetic objects that includes antiskyrmions [265], merons, bimerons, etc, all featuring various forms of chiral magnetic textures (see figure 22). Due to the nontrivial topology of their spin texture, these skyrmions are expected to be very stable [266, 267], can have a diameter of only few nanometers, and are in principle very easy to manipulate by tiny electrical and magnetic forces [268]. Thus, they hold real potential for future low-power and high-density magnetic memory and logic applications [269, 270], but also bio-inspired computing.

Magnetic skyrmions can emerge as a ground state, in which case they form a skyrmion lattice [262, 263] and collective behaviours become important, or as an isolated metastable state that can be manipulated individually.

Magnetic skyrmions were first experimentally observed in bulk non-centrosymmetric crystals [262, 263] and later on single ultrathin films [271]. Current approaches are largely centred on metallic heterostructures where a thin ferromagnetic layer is coupled to materials with large SOC. There, one can obtain skyrmions that are stable against perturbations of nanometer-scale size at room temperature. In these heterostructures, the key ingredient is the Dzyaloshinskii–Moriya magnetic interaction [272] (DMI) that emerges at interfaces upon the combination of broken inversion symmetry and strong spin–orbit interaction. Materials quality and interface control (Moriya–Dzyaloshinskii term) are key issues in skyrmions research that will allow controlling skyrmions properties in terms of size, shape, room temperature stability and mobility at low current densities.

Magnetic skyrmions can interact very efficiently with electrons and spin currents due to their non-collinear spin texture. This results in potentially high skyrmions mobility up to 1 km s^{-1} for current density of 10^8 A cm^{-2} .

Current and future challenges

Although the magnetic skyrmions possess great potential for applications, there are several challenges related to materials quality and interface control, spin sensitive imaging techniques and theoretical modelling. Any utilization of skyrmions in future technological applications will require room temperature all-electrical generation, manipulation, and detection of individual skyrmions.

Magnetic skyrmions can be generated by magnetic and electric fields, electric current, thermal gradients, or geometrical constrictions from domain walls. Here the challenge is to obtain better deterministic nucleation, both in space and time. The manipulation of skyrmions presents at least two challenges. One is related to the improvement of the spin-torque induced motion of skyrmions to obtain large skyrmion velocities. To do so, one can use materials with larger efficiency than heavy metals to produce spin currents such as Rashba/Dirac/valley–Zeeman interfaces. The second challenge is related to the presence of the skyrmion Hall effect that can create an undesired oblique skyrmions motion [264]. Using narrow nanowires could be a way to mitigate this problem, although skyrmions tend to vanish when reaching the wire's boundary. An alternative route is to use synthetic or real antiferromagnets, where the oblique motion is naturally suppressed [273]. There, the challenge is however to control the lateral expansion occurring at high velocity [274].

For detection, recent works have focused on the electrical read-out of skyrmions by exploiting the characteristic magneto-transport (the conventional type of read-out scheme based on the TMR effect, the anomalous Hall effect), the topological Hall effect, or magnetoresistance effect measured with an STM non-magnetic tip, although the latter seems unpractical for industry.

Despite its substantial success in terms of skyrmion nucleation and manipulation, a reliable and all-electrical design integrating electric write-in, transmission and read-out of magnetic skyrmions remains a

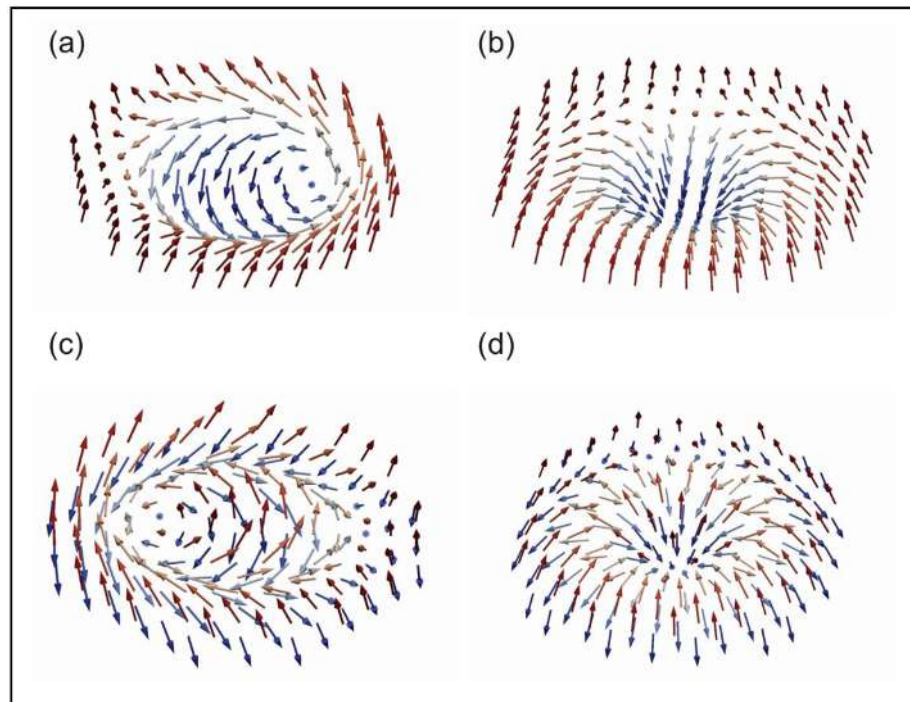


Figure 22. Typical skyrmion spin textures where the spin texture is indicated by the arrows. (a) Bloch-type skyrmion; (b) Neel-type skyrmion; (c) Bloch-type antiferromagnetic skyrmion; (d) Neel-type antiferromagnetic skyrmion.

challenge. Two possible concepts exist to solve this hurdle; using the STT based-switching by vertical spin-polarized current injection and/or using a local electric-field effect. The use of local electric fields to create and delete individual skyrmions offers dissipation-less alternatives, compared to STT, for energy efficient skyrmion devices (see figure 23).

In addition to being very attractive for technological applications, magnetic skyrmions exhibit novel phenomena such as topological and skyrmion Hall effects [264]. Future research might help to understand the dynamics of skyrmions and to account for quantum and lattice effects. These rich phenomena can include Bose–Einstein condensation, localization, Mott–superfluid transition or Wigner crystallization.

Advances in science and technology to meet challenges

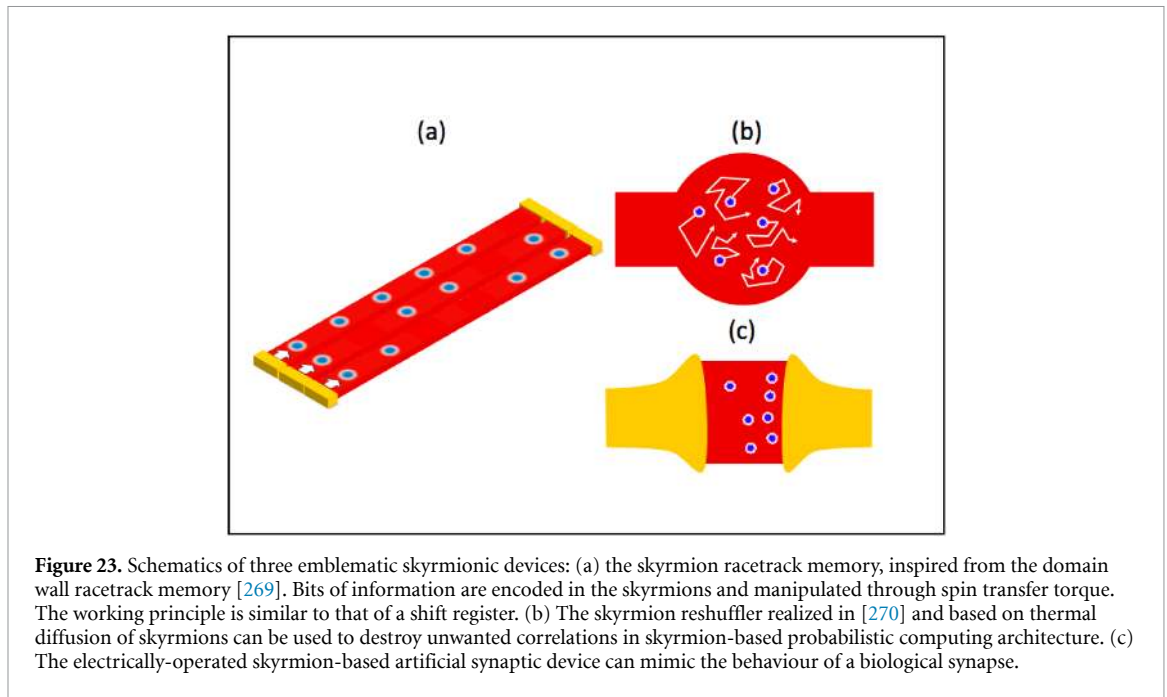
For progress to continue, substantial improvement in the understanding and control of various aspects of magnetic skyrmions are required.

For high-density and fast magnetic memory applications, very small (\sim nm) and high mobility (1 km s^{-1}) skyrmions are necessary. Due to their nontrivial spin texture, electrons flowing through skyrmions experience a fictitious magnetic field (order of 100 Tesla) that increases upon scaling down the skyrmion size and leads to topological and skyrmion Hall effects. Hence, small skyrmions are expected to display deteriorated transport properties. A better understanding of this effect is necessary to understand the edge motion of the skyrmions and identify efficient electrical detection methods.

Small and fast skyrmions require advanced engineering of ferromagnetic multilayers (to better control of the interlayer dipolar fields) but also novel structures based on synthetic ferrimagnetic and synthetic antiferromagnetic multilayers [275]. In addition, since skyrmions belong to a large family of chiral magnetic objects, the search for novel paradigms with different properties, e.g. the antiskyrmions, could open new perspectives (absence of Hall effect, better topological protection).

Another beneficial direction is the interaction between skyrmion and thermally and electrically excited magnons. Together with a detailed study of skyrmion–skyrmion and skyrmion–anti-skyrmion interaction that could lead to the design of devices with high skyrmion mobility and novel ways of deleting/annihilating skyrmions.

To take advantage of their huge potential for technological applications, multilayers engineering, new device design, novel materials, and advanced inspection techniques will be highly desirable. To characterize nm size skyrmions, as well as their dynamics and their spin texture high-resolution microscopy techniques such as but not limited to x-ray methods, advance electron and nitrogen-vacancy centre microscopy will be required.



On the materials side, as an alternative, one can envision the use of 2DMs, such as vdW magnets [276], graphene, TMDC or their combinations i.e. vdW heterostructures with several advantages. Strong SOC plays a central role in these systems. For example, in vdW magnets SOC stabilizes the perpendicular magnetic anisotropy, in graphene/TMDC interfaces SOC can efficiently generate spin currents via the Rashba and Zeeman valley couplings [13]. These couplings can favour small size skyrmions with high mobility. Graphene can be used as alternative to detect skyrmions. Graphene is sensitive to the properties of the substrate on which it is placed and can inherit substrate properties due to proximity effect.

Concluding remarks

Magnetic skyrmions bring nanometre-scale information size, stability against external perturbations, high speed and performance advantages beyond the theoretical limits of conventional magnetic technology. Rapid advances have been achieved in materials engineering and experimental design that allowed nucleation, manipulating and deleting individual skyrmions. Novel skyrmion devices concepts have been proposed such as racetrack type memory applications, logic devices, skyrmion oscillator, bio-inspired devices, topological based communication and computing designs.

For the future, it will be necessary to substantially advance the understanding and control of the interaction between skyrmions and the interaction of skyrmions with spin currents and magnons. Advance in materials engineering allowing generating nm-size skyrmions that are stable at room temperature and easily manipulated with tiny currents or local electric fields together with advanced imaging methods for the study of spin texture and dynamics skyrmions would be needed. The discovery of novel chiral magnetic objects beyond skyrmions with improved properties will undoubtedly facilitate the translation towards industrial applications. Their special topological properties would allow us to explore fascinating new physics in ways not possible with other particles. More important, given the technological importance of non-volatile magnetic memories today, the research on magnetic skyrmions will continue at least at a similar rate and level.

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15. Machine learning using experimental quantum materials data

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Status

The central goal of modern quantum materials is to search for new systems and technological paradigms that utilize quantum mechanical aspects of matter rather than being limited by them. In particular, there is an active search for new materials that exhibit surprising physical properties because of strong correlations. The key challenge in discovering these new materials lies in understanding strongly correlated quantum matter that defies both the simple theory and the majority of *ab initio* computations. Hence any progress has generally been experimentally driven. Decades of efforts in developing new experimental techniques and improving the resolution of instruments and detectors put us in an abundance of complex and comprehensive data. Two particular frontiers are (1) ‘image’-like real space data obtained through scanning tools and (2) high-dimensional and voluminous momentum space data obtained through scattering tools. The next breakthrough in the field will come from relating vast quantities of collected experimental data to theoretical models using tools of data science.

Current and future challenges

Increasingly, data science tools such as ML are showing great promise for accelerating discovery of materials through guided searches [27, 277–279] and for improving our understanding of simulated synthetic data associated with key models [280–283]. The next challenge is to tackle the data-driven challenges forming the critical bottlenecks between comprehensive and complex experimental data on quantum materials and a theoretical understanding. Although these data-driven challenges require a fundamentally new data science approach for two reasons: first, quantum mechanical imaging is probabilistic; and second, inference from data should be subject to fundamental laws governing microscopic interactions. Hence the readily-available data science tools need to be suitably altered to comply with hard and fast rules of fundamental microscopic laws. Moreover, any insight from learning by machines require ‘sanity check’ or ‘interpretation’ on machine’s learning [284].

Advances in science and technology to meet challenges

Recently significant first steps were taken towards matching complex experimental data such as ‘image’-like data to theoretical hypothesis, discriminating multiple hypothesis against each other and hence offering theoretical insight, using ML [285, 286]. In Ref. [283], we have developed and demonstrated a new general protocol for ML-based identification of symmetry-breaking ordered states in electronic-structure images. Our artificial neural networks were trained to learn the defining motifs of each category, including its topological defects, and to recognize those motifs in experimental data (figure 24). Applied to the hole-doped Mott insulator state harbouring the enigmatic pseudogap states [92] over a wide range of doping, the neural networks repeatedly and reliably discovered the predominant features of a specific ordered state of unidirectional period $4a_0$ density wave modulations at the pseudogap energy that break the global rotational symmetry to generate a nematic state (see figure 25). Hence the ML based hypothesis testing revealed that strong coupling mechanism that drives such commensurate order is universally at play in the entire underdoped regime of the cuprate phase diagram. In [284], we showed that the modality developed in [283] readily extends to a completely different measurement technique of resonant ultra-sound spectroscopy.

Concluding remarks

The demonstrations that artificial neural networks can process and identify specific broken symmetries of highly complex experimental image arrays [283] and constrain the nature of order parameter from a sequence of peaks [284] are milestones for general scientific techniques. Moving forward, more progress in unsupervised discovery from high-dimensional and voluminous momentum space data are to be much anticipated.

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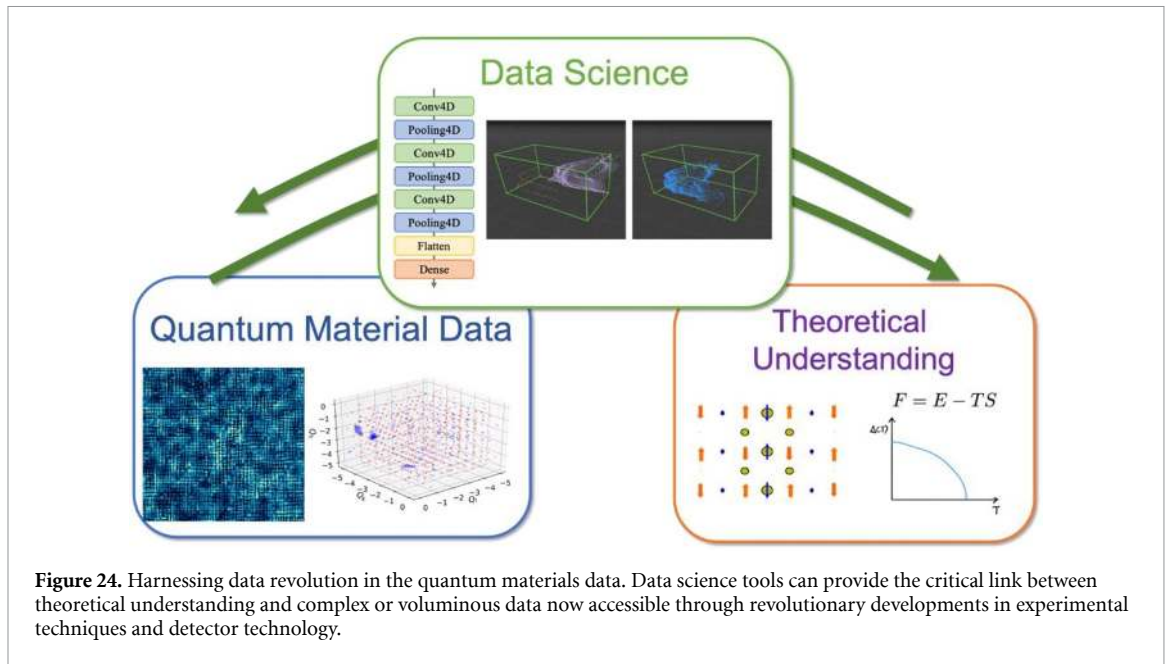


Figure 24. Harnessing data revolution in the quantum materials data. Data science tools can provide the critical link between theoretical understanding and complex or voluminous data now accessible through revolutionary developments in experimental techniques and detector technology.

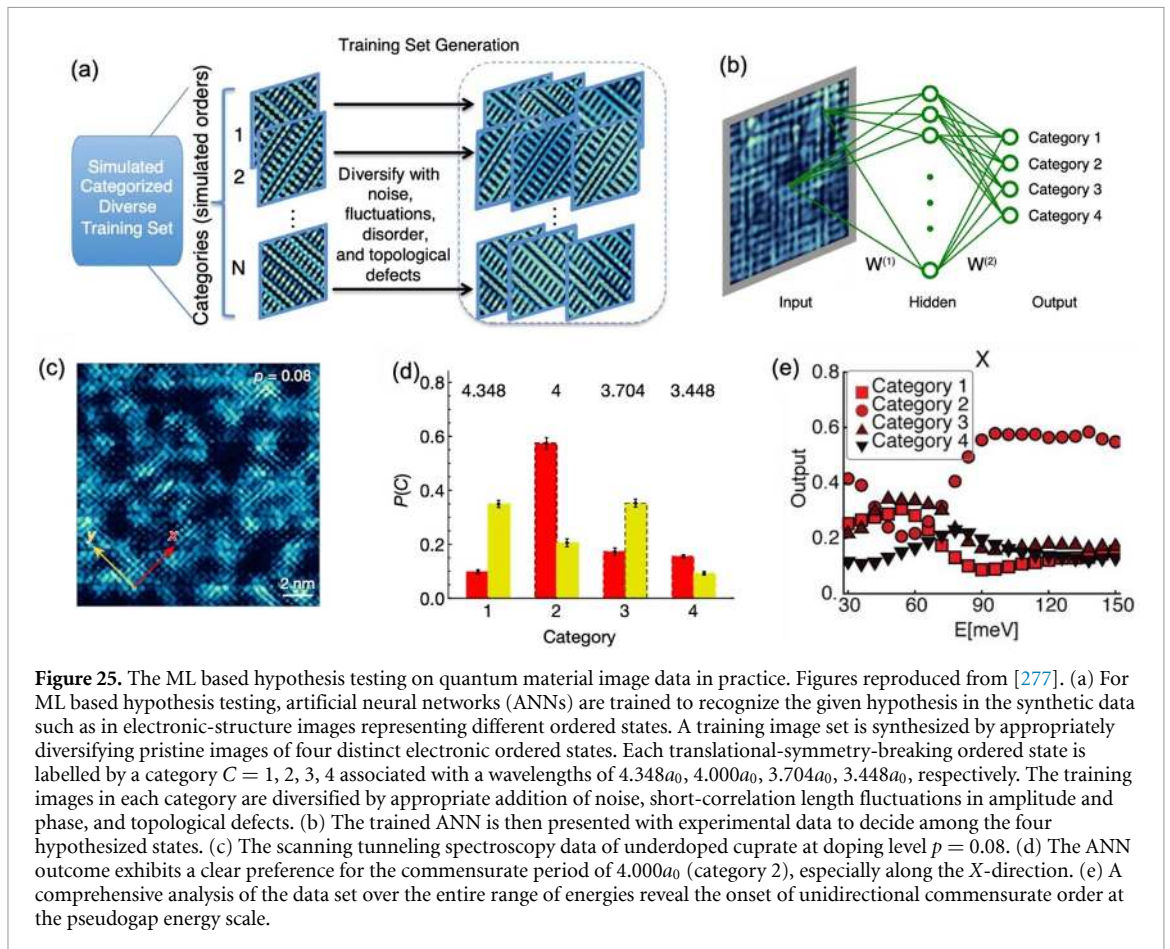


Figure 25. The ML based hypothesis testing on quantum material image data in practice. Figures reproduced from [277]. (a) For ML based hypothesis testing, artificial neural networks (ANNs) are trained to recognize the given hypothesis in the synthetic data such as in electronic-structure images representing different ordered states. A training image set is synthesized by appropriately diversifying pristine images of four distinct electronic ordered states. Each translational-symmetry-breaking ordered state is labelled by a category $C = 1, 2, 3, 4$ associated with a wavelengths of $4.348a_0, 4.000a_0, 3.704a_0, 3.448a_0$, respectively. The training images in each category are diversified by appropriate addition of noise, short-correlation length fluctuations in amplitude and phase, and topological defects. (b) The trained ANN is then presented with experimental data to decide among the four hypothesized states. (c) The scanning tunneling spectroscopy data of underdoped cuprate at doping level $p = 0.08$. (d) The ANN outcome exhibits a clear preference for the commensurate period of $4.000a_0$ (category 2), especially along the X-direction. (e) A comprehensive analysis of the data set over the entire range of energies reveal the onset of unidirectional commensurate order at the pseudogap energy scale.

16. Machine learning and DFT simulations of quantum materials

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Status

The microscopic understanding of materials started with the paradigm shift from Classical to Quantum Mechanics in the early 20th century. Based on Schrödinger and Dirac equations, the accurate description of the behaviour of materials at the fundamental level was for the first time possible. This enabled the understanding of many phenomena that were not possible until then. Although in principle any problem can be described by quantum mechanics, in practice, even for simple cases this is not possible due to the complexity in solving the many-body problems. One example is superconductivity, which was discovered in 1911 but explained only 46 years later. This led to the famous Dirac remark in 1929 stating that *the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved*. This remark precludes the imminent central role of Computational Materials Science, presenting the main technical challenges for it to overcome.

With the impressive computational advances both in methodologies and technologies, especially since the 1970s, the description and simulation of realistic quantum materials have been possible. DFT established itself as the standard tool for simulation of materials systems after success in describing many important physical properties such as ground state structures, relative total energies, and electronic band structures. Subsequently, major milestones were achieved such as the description of structural, electronic, optical, magnetic, catalytic, and quantum properties, both for bulk and nanoscale materials.

Nowadays, with the ever-increasing data generation, including high-throughput techniques [287], and storage from sources as diverse as imaginable, and with the developments in computational and information science, a new data-driven paradigm has emerged (figure 26(a)). Building from experimental, theoretical, and computational science paradigms, the data-driven science paradigm aims to extract knowledge from this huge amount of raw data and information now available [288]. In practice, data-driven science is embodied in novel tools and algorithms; among those, the field of statistical learning developed Machine Learning (ML) techniques, which are increasingly important [28]. These algorithms generate output results given any kind of numerical input data, whether theoretical or experimental. In materials research, many kinds of problems have been tackled, and different strategies have been thought. These can be broadly classified into learning properties of three types (figure 26(b)): (a) pre- Schrödinger equation, such as learning the electronic density [289], to be then used as input for DFT or ML; (b) replacing- or accelerating- Schrödinger equation, thus creating machine-learned approximations to solving the quantum problem; and (c) post-Schrödinger equation, such as directly learning the outputs of the problem, as structures, energies, and materials properties. Examples include the discovery of novel 2DMs and properties [290], learning and predicting novel topological materials [291, 292], and creating a twistrionics database for identifying strongly correlated behaviour in 2D systems [293].

Current and future challenges

Two main materials science goals are (a) materials design/optimization (local search or exploitation), and (b) materials discovery (global search or exploration). The first aims to find among all known materials, the best candidates for each interest property or application, and then how to improve promising and interesting systems further. The second aims to discover the maximum number of novel materials, exploring simultaneously the atomic (elements), compositional (stoichiometries), and configurational (geometries/structures) spaces. As such, the number of degrees of freedom is immense, and the search (sampling) strategy in this space is of paramount importance.

Currently, both goals present major challenges. The traditional direct approach (a) includes ever-increasing complex properties such as magnetism, topology, superconductivity, and many others where quantum and many-body effects are of extreme importance. As such, on the technical side, more complex calculations demand progressively more computational power, also allowing for larger realistic systems to be treated. Challenges present for implementing sufficiently higher-level theories needed to account for quasiparticle and many-body interactions, simultaneously with computational efficiency for required system sizes. Fundamental challenges also present in developing DFT functionals better-describing correlation effects. In certain cases, the development of the fundamental theoretical framework can itself be a challenge, such as the aforementioned superconductivity description.

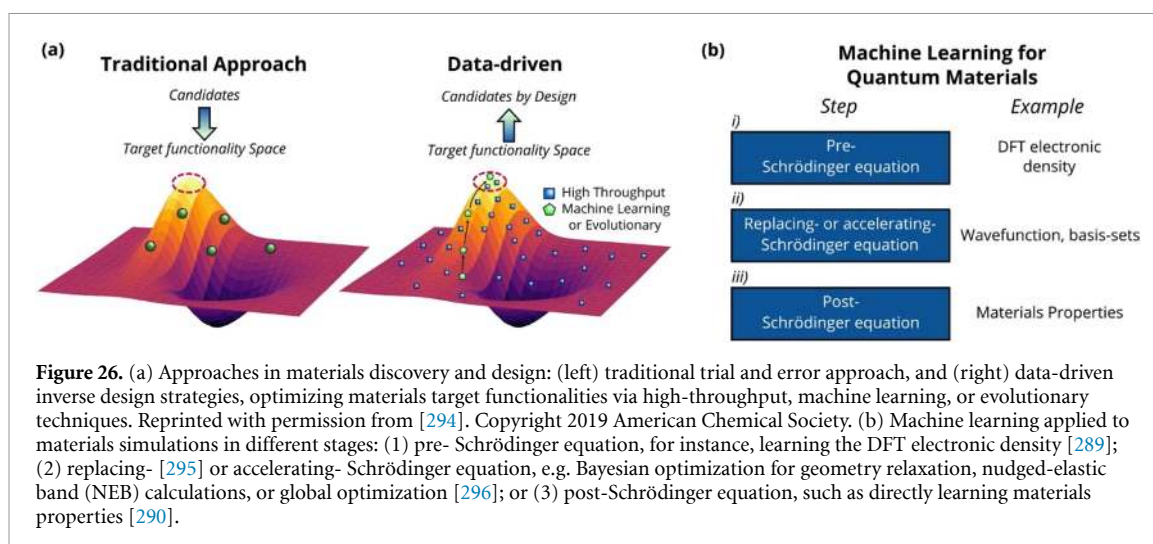


Figure 26. (a) Approaches in materials discovery and design: (left) traditional trial and error approach, and (right) data-driven inverse design strategies, optimizing materials target functionalities via high-throughput, machine learning, or evolutionary techniques. Reprinted with permission from [294]. Copyright 2019 American Chemical Society. (b) Machine learning applied to materials simulations in different stages: (1) pre-Schrödinger equation, for instance, learning the DFT electronic density [289]; (2) replacing- [295] or accelerating- Schrödinger equation, e.g. Bayesian optimization for geometry relaxation, nudged-elastic band (NEB) calculations, or global optimization [296]; or (3) post-Schrödinger equation, such as directly learning materials properties [290].

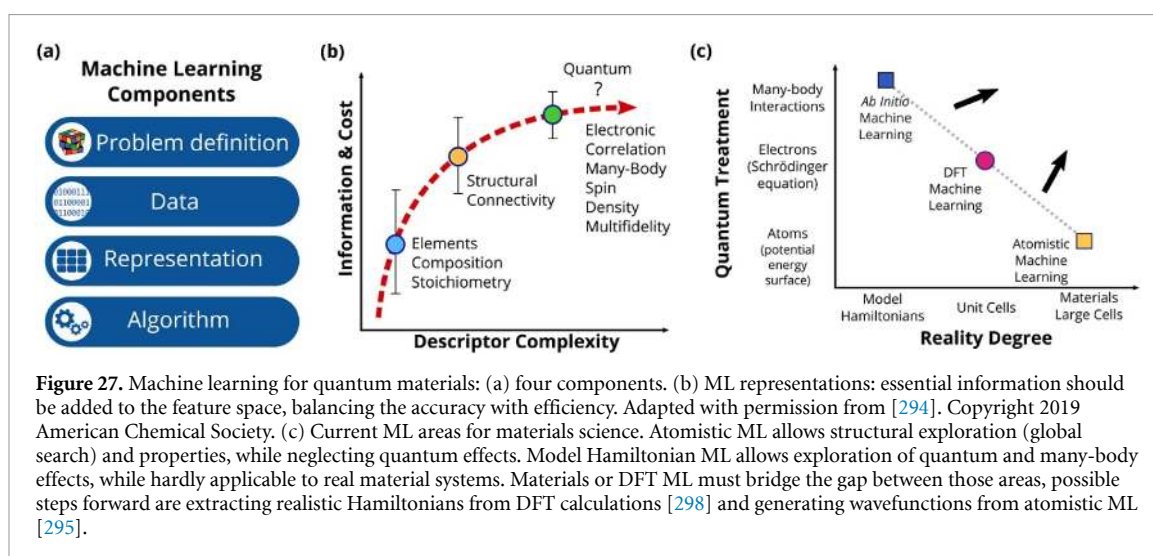


Figure 27. Machine learning for quantum materials: (a) four components. (b) ML representations: essential information should be added to the feature space, balancing the accuracy with efficiency. Adapted with permission from [294]. Copyright 2019 American Chemical Society. (c) Current ML areas for materials science. Atomistic ML allows structural exploration (global search) and properties, while neglecting quantum effects. Model Hamiltonian ML allows exploration of quantum and many-body effects, while hardly applicable to real material systems. Materials or DFT ML must bridge the gap between those areas, possible steps forward are extracting realistic Hamiltonians from DFT calculations [298] and generating wavefunctions from atomistic ML [295].

In the inverse approach (b), i.e. the search for materials presenting certain desired functionalities, exploration of the large materials space is fundamental. Therefore, high-throughput, evolutionary, and ML techniques are increasingly important to efficiently sample the materials space, resulting in screened cases for in-depth investigation. High-throughput approaches present challenges regarding the construction of consistent databases for expensive calculations, unfeasible to be performed exhaustively [297]. Although successful, ML approaches require four interdependent components (figure 27(a)), each demanding careful examination and presenting its own challenges: (1) *problem definition*, (2) *data (inputs)*, (3) *representation*, and (4) *algorithms* and model training.

Advances in science and technology to meet challenges

Advances in both materials science goals—materials discovery and design—mutually benefit. Beyond traditional manual developments, artificial intelligence and ML techniques can be broadly employed, improving every problem-solving steps. This includes estimating the computational cost [299], optimizing simulation and parallelization parameters for faster and numerically efficient calculations, creating optimized density functionals, obtaining information for use or directly bypassing simulations, and directly obtaining results and materials properties.

Toward this, ML advances in each of its components are needed. First, quantum materials ML *problem definition* might be supervised, i.e. regression of a numerical property or classification among different categories. If on the other hand, an exploratory and unbiased approach is more suitable, unsupervised tasks such as dimensionality reduction and clustering techniques can be preferred. Regarding *input data*, quantum materials generally allow for the creation of smaller databases, in contrast to big-data datasets. Accordingly, the representation used and the algorithm to be employed must also be carefully selected. Merging experimental and literature-extracted data can be valuable [300], with the additional benefit of improving

agreement to experiments, as also using multi-fidelity, data augmentation, and transfer learning techniques. Certainly, the *representation*, also called ‘descriptor’ or ‘fingerprint’, is the central element in ML for quantum materials, where nonlocal, collective, and many-body effects need to be accounted for. The challenge is distilling the fundamental information from the systems into efficient numerical descriptions (figure 27(b)). Insights can be taken from two more mature ML areas (despite having larger datasets): atomistic potential energy surface ML, and many-body Hamiltonian ML (see Roadmap section ‘ML using experimental quantum materials data’). The first usually uses additive descriptions based on local atomic environments, while the latter succeeded by translating Hamiltonians into image-like vectors or tensors commonly used with deep neural networks. Developments for quantum materials lie between these two areas, i.e. describing quantum phenomena in realistic systems, with ML as a driver for advances (figure 27(c)). Lastly, the *algorithm* choice must suit the problem data size and representation, for instance, deep learning can have hundreds to millions of trainable coefficients which is unreasonable for small datasets.

Finally, exciting advances are expected in the area of distilling the data-driven correlation models for driving theoretical understanding of studied problems. Interpretability of generated ML models is a first step in this direction, but progress toward physics-enhanced surrogate models [290, 301], and the broader goal of machine-assisted discovery of underlying fundamental physics [302] is essential. In practice, it is crucial to incorporate ML strategies into routine workflows, whether by direct integration into used software or as interoperable standalone software libraries.
















Concluding remarks

Computational physics has traditionally been at the core of many fundamental advances related to quantum systems and materials. With the development of computational methodologies and high-performance computing and storage technologies, this progress has enabled more and realistic problems to be treated with ever-increasing levels of theory. State-of-the-art DFT has driven the field forward, but it faces challenges to overcome. The expansion in information-generation capability is ideal for data-driven approaches such as machine and deep learning, which can accelerate or make possible knowledge production for the different complex problems related to quantum materials. Challenges exist related to problem definition, data acquisition, efficient and complete representations, and suitable algorithms to be used. The field is still in its beginning, and many opportunities lie ahead for future developments.

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