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The 2022 applied physics by pioneering women: a roadmap

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Roadmap

The 2022 applied physics by pioneering women: a roadmap

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Abstract

Women have made significant contributions to applied physics research and development, and their participation is vital to continued progress. Recognizing these contributions is important for encouraging increased involvement and creating an equitable environment in which women can thrive. This Roadmap on Women in Applied Physics, written by women scientists and engineers, is intended to celebrate women's accomplishments, highlight established and early career researchers enlarging the boundaries in their respective fields, and promote increased visibility for the impact women have on applied physics research. Perspectives cover the topics of plasma materials processing and propulsion, super-resolution microscopy, bioelectronics, spintronics, superconducting quantum interference device technology, quantum materials, 2D materials, catalysis and surface science, fuel cells, batteries, photovoltaics, neuromorphic computing and devices, nanophotonics and nanophonics, and nanomagnetism. Our intent is to inspire more women to enter these fields and encourage an atmosphere of inclusion within the scientific community.

Keywords: pioneering, women, applied physics

(Some figures may appear in colour only in the online journal)

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Introduction

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Women have long made important contributions to applied physics. A few notable examples among many include pioneering research on radioactivity by Marie Curie, x-ray crystallography of the structure of DNA by Rosalind Franklin, the discovery that parity is not conserved in particle physics by Chien-Shiung Wu, investigations of layered and magnetic semiconductors by Shirley Ann Jackson, advances in carbon-based low dimensional structures by Mildred Dresselhaus, and the development of chirped pulse amplification to enable intense ultrafast lasers by Donna Strickland. Untold additional contributions, large and small, have also produced critical building blocks and breakthroughs. At a time when applied physics needs contributions from the brightest minds, more than ever we need to ensure that women are increasingly involved across a wide range of disciplines to embrace the full human potential.

Many studies and working groups have concluded that science benefits from a deeper, more diverse workforce, particularly considering the contributions of women [1]. The number of women participating in applied physics research has historically trailed that of their male counterparts across the globe, although the absolute degree varies by country and sub-discipline. Several factors have been linked to the lower-than-desired involvement of women in these fields, including lower pay, lower rates of promotion, inadequate parental leave support, insufficient mentorship, fewer resources and persistent, but subtle, micro-aggressions in the workplace. We note that while we have elected to focus on women here, these arguments hold for diversity across race, ethnicity, nationality, sexual orientation, (dis)ability and other identities. Such factors are often further compounded for women who are also part of these other underrepresented minority groups.

This introduction aims to set the context and reason for such a roadmap. It does not aim to provide a fulsome review of the research, statistics and programs that consider addressing the low numbers of women in applied physics. Rather, to better understand and address these core issues, we acknowledge that many working groups and initiatives have been established, including the International Union of Pure and Applied Physics Working Group 5 on Women in Physics, the Association of Asia Pacific Physical Societies Working Group on Women in Physics, the American Physical Society Women in Physics and the African American

Women in Physics, the Science in Australia Gender Equity, and Athena SWAN (Scientific Women's Academic Network) in the United Kingdom. A review of actions is given in [2]. We support these organized efforts and encourage their work to continue.

Their research has uncovered some stark data and information. The most pressing concern is that the percentage of women in post-graduate physics positions has stalled at just below 20% internationally [3]. The American Institute of Physics has tracked the representation and participation of women in physics with several global surveys [4] and has identified that unequal resource distribution and parenting have long-term effects on women's careers [5].

However, additional programs can have impact at the grassroots level. One of them is recognizing the scientific accomplishments of women. Such actions can achieve impact for two reasons: it helps to create an equitable environment where everyone is fairly treated, and it makes the work of women scientists more visible, which can drive further participation. Role models and examples of success help to demonstrate that scientific careers are attainable and desirable. As the adage goes, 'you cannot be what you cannot see'. When consistently applied over time, this approach can have a compounding effect. Recognition is therefore a powerful and readily available tool for increasing diversity, equity and inclusion in science [6].

This roadmap on Women in Applied Physics, written by women scientists and engineers, is intended to celebrate contributions women have made across 15 sub-disciplines that are representative of current interests within the applied physics community. Space constraints prevent us from highlighting every deserving topic or accomplishment, but our goal is to present examples of impactful work that may inspire others. Each sub-discipline has contributions by experienced and earlier career researchers—examples of rising stars—as we aim to showcase the stages of contributors along the career pipeline.

In line with our aim to embrace diversity, each sub-discipline author approached their section in their own way to celebrate and highlight examples of research activities by women.

This roadmap is also intended to encourage others to help accelerate efforts to improve women's participation in applied physics disciplines. By recognizing women's accomplishments, we are providing evidence of why we must increase the inclusion of women in conferences, on boards and in decision-making processes and take steps to break through the current plateau to build the number of women in physics.

We commend the focus that the IOPP has on addressing women in physics for not only supporting this roadmap but also their requirement for gender quotas on editorial boards and as referees.

Finally, we must appreciate that we all (men and women) have the capacity to act as mentors and agents of change. In

addition to their extensive scientific output, women physicists like Chien-Shiung Wu and Mildred Dresselhaus worked tirelessly as advocates for and mentors to women scientists. However, women cannot shoulder this burden alone. We each can do our part in small and large ways to help bridge the gap in women's participation in applied physics.

This roadmap is one step to redress the low numbers of women in applied physics by showcasing and celebrating the world-class research undertaken by women in these 15 sub-disciplines. We hope this will inspire you to redouble efforts to recognize the accomplishments of women and increase inclusion so that we can embrace the full human potential!

1. Plasma materials processing

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Status

The fascinating science of plasma as the fourth state of matter manifests itself through diverse applications ranging from plasma fusion to materials processing and treatment of living matter. Whereas material processing by thermal plasma has found major applications in the field of metallurgy for decades, with contributions from scientists such as Armelle Vardelle (University Limoges, FR), low-temperature plasma⁴⁶ has given rise to several and diverse applications and it will be the focus of this section. Historically (see figure 1), low-temperature plasma has been of paramount relevance in the field of microelectronics, where the fabrication is ruled by thin-film deposition and material etching steps, with remarkable achievements of women [7]. Here, we acknowledge the major contributions of Frances Houle (LBNL, USA), Jane Chang (UCLA, USA), Ellen Fisher (University New Mexico—ex Colorado State University, USA), who delineated plasma–surface interactions in silicon-based etching processes, while Karen Gleason (MIT, USA), Bogdana Mitu (INFLPR, RO), Agnes Granier (University Nantes, FR), Farzaneh Arefi-Khonsari (Sorbonne University, FR), and Marcela Bilek (University Sydney, AU) led the development of plasma-assisted materials synthesis, including polymers and biomaterials. Knowledge of electron-impact-induced molecule dissociation towards radical production, their surface reaction probability (sticking/recombination), and the flux and energy of the ions accelerating through the plasma sheath towards the substrate's surface is highly relevant to master the thin-film properties sized to specific applications or to promote (an-)isotropic and selective material etching (see figure 2) [8, 9]. In parallel, the non-equilibrium character of low-temperature plasmas has progressively been explored [10], primarily under atmospheric pressure, in other research fields because the temperature budget is compatible with sensitive materials. In this respect, we consider the pioneering work of Satiko Okazaki (Sophia University,

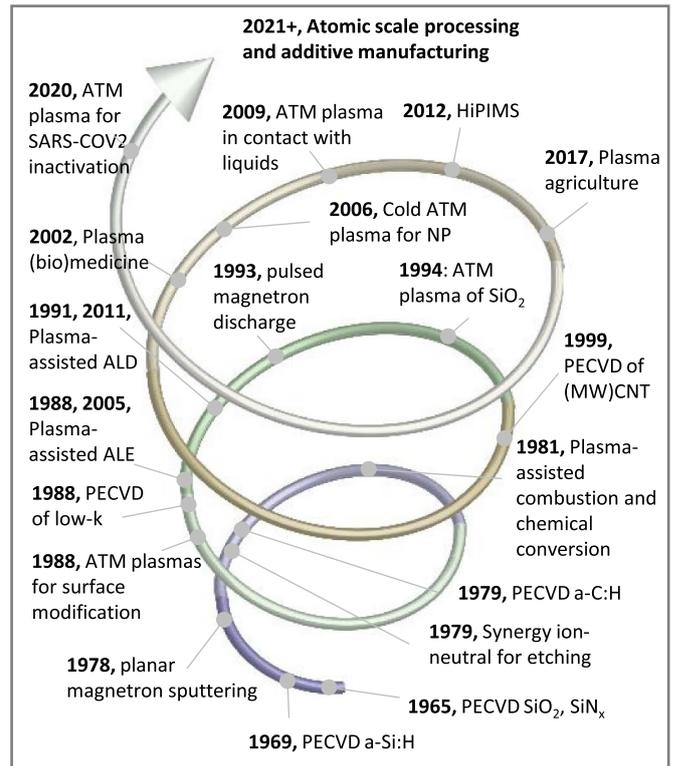


Figure 1. Overview of the historical advances in materials processing with low-temperature plasmas.

JP), Françoise Massines (CNRS PROMES, FR), and Hana Barankova (Uppsala University and BB Plasma Design AB, SE) in various atmospheric pressure plasma configurations, followed by the development of applications by Daphne Pappas (Plasmatreteat USA) and Fiorenza Fanelli (University di Bari Aldo Moro, IT). For plasma interactions with living matter, two selected highlights are the fields of plasma agriculture [11], embracing water cleaning and treatment of seeds and plants, and plasma medicine through the use of micro-plasmas, addressing applications such as wound healing, sterilization, dermatology and dentistry [12]. Noteworthy are the works of Nevena Puač (Inst. of Physics Belgrade, RS) in plasma agriculture and those of Selma Mededovic Thagard (Clarkson University NY, USA) and Monica Magureanu (INFLPR, RO), who depollutes water by plasma degradation of polyfluorocompounds/pharmaceuticals/pesticides. In parallel, the field of plasma medicine initiated by Eva Stoffels-Adamowicz (Marmelot—Maru-vet Ltd) was strongly developed around the world by prominent scientists like Deborah O'Connell (Dublin City University, IR) and Cristina Canal (University Politecn. Catalunya, ES), working on cancer treatment, Kiwon Song (Yonsei University, KOR), evidencing the regenerative capabilities induced by plasma treatment, and Graciela Brelles-Mariño (University Nac. La Plata, AG), proving biofilm inactivation by plasma and demonstrating strong interdisciplinarity among physics, chemistry, biology and medicine. More recently, the field of nanoelectronics exploits the synergy between low-temperature plasma and atomic layer deposition (ALD)/etching [13], bringing in the self-limiting

⁴⁶ Material processing is generally carried out under low-temperature plasma conditions, where the electron density is in the range of 10^9 – 10^{10} cm⁻³ and the ionization degree is in the range of 10^{-6} – 10^{-3} . Electrons have temperatures as high as 5×10^3 K– 10^5 K (from tenths to a few eV), whereas ion/gas temperatures are in the range of 300 K–500 K.

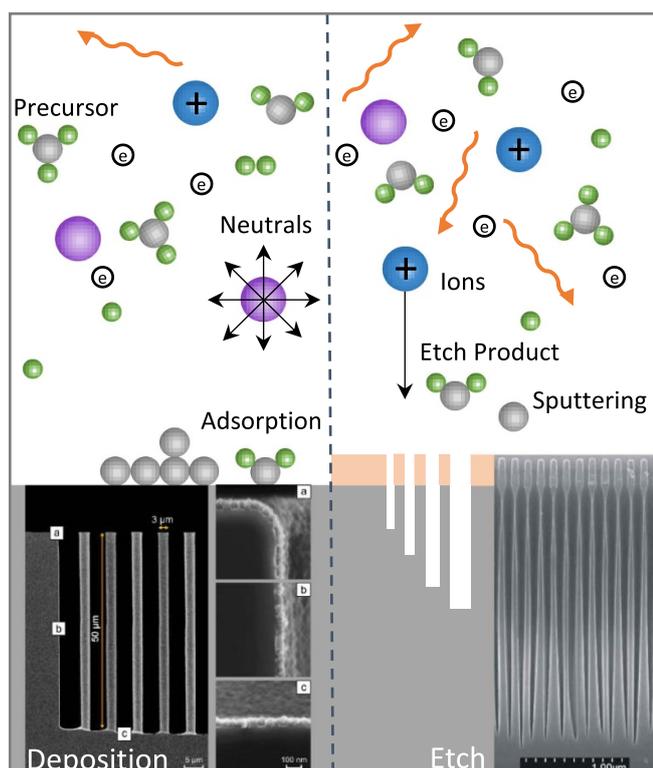


Figure 2. The interplay between plasma species and surfaces enables complex surface topography in materials processing. Reproduced from [17]. CC BY 3.0. Reprinted from [18], with the permission of AIP Publishing.

character of gas–surface reaction processes and material selectivity. Keren Kanarik (Lam Res. Corp., USA) elucidated fundamental reaction pathways enabling atomic layer etching of materials and Mariadriana Creatore (TU/e, NL), Ageeth Bol (University Michigan, USA) and Jolien Dendooven (Ghent University, BE) developed a plasma-based ALD process for material synthesis.

Current and future challenges

The future research on low-temperature plasma processing knows practically no boundaries, but opportunities and challenges. This is definitely the case of plasma processing of beyond-silicon materials, atomic-to-nano fabrication (defects and roughness at atomic scale, surface functionalization, nanoparticles or nanocomposites), and plasma processing on chemically (hybrid (in-)organic chemistry) and physically (high aspect ratios, high internal surface area) challenging substrates for energy conversion and storage applications. Timely applications are, in this respect, metal halide perovskite photovoltaics (PV), (3D) solid-state batteries, (photo)electro-catalysis and CO₂ capture and storage [14]. Equally intriguing is the application of plasma in catalysis, aiming to contribute to the major goal of electrification of the chemical industry. Steering chemical processes requires insights into how electron energy can be channeled (via selected vibrationally and electronically excited modes) to lead to selective and efficient chemical

reactions and on the interaction between plasma and catalyst (photons, ion bombardment, surface charging, hot spots).

In general, the adoption of plasma enables overcoming certain thermodynamic and kinetic limitations that are observed for thermally based chemical reactions. The overarching goal is to tailor the chemical specificity and allow for the control of reaction selectivity. However, the fact that a very large number of reactive species (photons, ions, electrons, radicals, excited molecules) are generated with a plasma often makes it difficult to delineate individual effects [15]. Therefore, it is becoming increasingly important to combine complementary *ab initio* calculations that can elucidate detailed reaction mechanisms that are inaccessible otherwise, multi-scale modeling that bridges the time/length scales of surface reactions, and state-of-the-art spectroscopy and metrology that enable experimental validation [16]. Often, individual research groups focus on one aspect of these efforts and strong collaborations (national and international) are needed to accomplish these goals.

Advances in science and technology to meet challenges

All the above-mentioned (and many more) plasma applications share the same scientific challenge of understanding and governing plasma–surface interactions, with vital contributions from sensitive diagnostics and computational efforts. Advances have been made in the investigation of plasma species, their energy and reaction kinetics through measurements, and numerical modeling and simulation by the groups of Annemie Bogaerts (University Antwerp, BE), Kinga Kutasi (Wigner Res. Center Phys.—ex Acad. Sci., HU) and Amy Wendt (University Wisconsin Madison, USA). The combination of all the above-mentioned approaches is proving to be the key towards understanding both the fundamentals and the practical aspects of plasma materials processing.

The implementation of several and complementary diagnostics of plasma and plasma–surface interaction enables proper understanding of the influence of the chemical and physical aspects of plasma species on their density and directionality towards the processed surface. Especially in the case of nanoscale processing, the effect of strong discontinuities (electrical, chemical and thermal) on the edges should be understood in terms of plasma physics and chemistry, and translated and leveraged over desired properties at global scale. As such, modeling and simulation can prove their strength in providing valuable information on the sheath properties around these nanofeatures, as well as in the shadowed regions where diagnostics are almost impossible to implement, while new algorithms and codes would give the knowledge. *Ab initio* calculation is expected to be at the forefront of both plasma and material science developments. It has the power to calculate the rate coefficients needed for understanding plasma chemistry, as well as to ‘invent’ new materials as new combinations of elements and new system geometries. Only such holistic approaches could bring the solutions for the ever-growing demands of next-generation devices. Machine

learning capabilities where *ab initio* calculations might help in the design of experiments should be considered in the near future, while multiple diagnostics with real-time interpretation of the key parameters based on modeling, combined with active feedback on the reactions, would easily lead to ideal processing conditions.

A final consideration concerns the circularity of the problem/solution paradigm where understanding the physics and chemistry behind plasma processing and the development of new processes is dependent on the state-of-the art in electronics, while continuous advances in electronics rely on material processing, where plasma processing is often the limiting step.

Concluding remarks

Low-temperature plasma processing science, due to its intrinsic non-equilibrium nature, has been and will continue to be at the heart of many key enabling technologies,

while providing breakthrough solutions in areas of human health, energy, and environmental sustainability. While climate change compels the research community to prioritize their current and future efforts towards Green Deal priorities, it is worth highlighting that plasma processing can be driven by renewable electricity resources and contributes to offering material processing approaches with low materials usage and energy consumption.

Identifying that common thread underlying various applications of plasma process science is challenging, yet it holds promise to augment beyond the ‘sum of the parts’, and to provide translational knowledge to enable technological breakthroughs and accelerate innovations by stronger interconnection of women from universities, research centres and industry. Let us leave no plasma nor materials behind and embrace distinct problems, different ideas, various approaches, diverse members, and above all, share common threads and lessons learned (both successful and unsuccessful) so we can make more progress.

2. Plasma propulsion

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Status

Plasma propulsion is the means by which ionized matter, under the influence of electric and/or magnetic fields, is accelerated to high velocities (typically in the range of tens of thousands of m s^{-1}) to produce thrust for spacecraft. Traditional space chemical propulsion systems use combustion to release energy stored in chemical bonds to heat a propellant, resulting in maximum exhaust velocities in the range of a few thousands of m s^{-1} . Plasma propulsion systems, which have been in use since the 1960s [19], are very efficient, and their higher propellant ejection velocities enable space missions using significantly less propellant than chemical propulsion counterparts. These mass savings facilitate the use of smaller launch vehicles, increased payload size, and more complex missions. This is an immense advantage for long-term space missions. In Earth orbit, plasma thrusters are used to maintain a satellite's orbit, overcome drag, change orbit, re-orient a satellite, and deorbit at end of life.

In recent decades, several notable milestones have been achieved in scientific missions relying on plasmas for primary propulsion, as summarized in figure 3. These missions have demonstrated the suitability of plasma propulsion for manoeuvres as varied as continuous drag compensation and asteroid landings. Maria Choi's (NASA Glenn Research Center) simulation work at NASA on plume interactions with spacecraft was integral to the organization's decision to begin using Hall effect thrusters (HETs) for scientific missions. NASA's first spacecraft with an HET will be the Psyche Mission, launching in August 2022.

There are now well over 200 satellites equipped with Electric Propulsion (EP) systems for various operations such as station keeping, orbit maintenance, orbit changes, space debris avoidance, insertion into graveyard orbits, and deorbiting [20]. Recently, constellations of thousands of satellites, such as Starlink, have used plasma propulsion to boost their initial 300 km orbit to over 500 km, where atmospheric drag is significantly lower [21].

All plasma propulsion systems rely on electrical energy to ionize and accelerate the propellant. Currently, all are solar-powered and limited by solar conversion technology and spacecraft size. To date, the highest-powered individual plasma propulsion unit used in orbit is a 5 kW class HET [20]. Systems that operate at more than 100 kW can produce significantly more thrust, and development of these systems

is vitally important for manned and cargo Moon and Mars missions. As the technology to produce more power in space advances, researchers are currently building upon pioneering magnetoplasmadynamic (MPD) thruster work by Monika Auweter-Kurtz (German Aerospace Academy, ASA). MPD technology offers very high thrust density; however, it requires a significant power input of at least 20 kW for efficient operation. In a different area of innovation, advancements in miniaturized satellites and CubeSats have introduced a plethora of small plasma thruster technologies focused on adding capability to a growing industry. Here, spacecraft size tends to be the limiting factor for power generation.

Current and future challenges

As plasma propulsion becomes more widespread, key challenges have arisen, including optimization of existing technologies, expansion of applications, and scaling in power and size. Constellations of thousands of satellites using plasma propulsion are creating the need for active debris removal and avoidance. Interesting physics related to off-nominal, higher thrust operation of plasma thrusters for debris avoidance is presenting new challenges. In addition, the general use of plasma propulsion on these constellations is transforming the development of plasma thruster systems from custom, single-mission needs, to mass production, with associated challenges and costs. Most plasma propulsion systems in operation are between 200 W and 5000 W and pose scaling challenges at the far ends of these power levels. Considerable innovation is being shown in laboratories around the world in developing plasma thrusters for small satellites and CubeSats. As the two most widely used plasma propulsion devices, gridded ion engines (GIEs) and HETs, scale down poorly in both size and power, efforts must be made to overcome this drawback.

Improving lifetime by limiting the wear of key thruster components in contact with plasma, and breaking away from empirical, prohibitively long and expensive thruster development methods, are priorities in current research. These are significant issues for existing technologies: as an illustration, qualification of NASA's new NEXT gridded ion thruster involved 22 000 h of operation at the highest throttling point. Telecommunications satellite constellations will require increasingly compressed timetables related to manufacture and life-testing under in-space conditions.

Significant ongoing research into the use of new propellants for EP systems, such as iodine and naphthalene (which sublimate at relatively low temperature and can be stored in solid form), to replace traditionally used compressed xenon and krypton, will make plasma propulsion more accessible for ride-share launch opportunities and small satellites. Ane Aanesland (ThrustMe) is a leader in the effort to make iodine-based plasma propulsion common. For very high-powered systems, lifetime determination remains a challenge. Vacuum facilities of sufficient size to handle the massive propellant throughput, power connections, and heat capacity are limited, and the cost of operating these facilities is extremely high. Fundamental plasma features, such as detachment from

Probe (operator)	Launch	Thruster	Objective	Milestones
Deep Space 1 (NASA/JPL)	1998	GIE	asteroid Braille and comet Borrelly flyby	first scientific mission to use plasmas as primary drive
SMART-1 (ESA)	2003	Hall	Earth-Moon mission	first scientific mission to use Hall thrusters as primary drive
Hayabusa (JAXA)	2003	GIE	Itokawa asteroid landing, sample recovery	first asteroid sample recovery
DAWN (NASA/JPL)	2007	GIE	study of protoplanets Ceres, Vesta	first plasma propulsion exploration mission
GOCE (ESA)	2009	GIE	Earth structure mapping	first extended drag compensation with ion propulsion
LISA Pathfinder (ESA)	2015	electrospray	proof of concept measurements for gravitational wave detection	validation of future LISA mission, first in-space gravitational wave observatory
BepiColombo (ESA/JAXA)	2018	GIE	Earth-Mercury mission	most powerful ion propulsion system flown to date

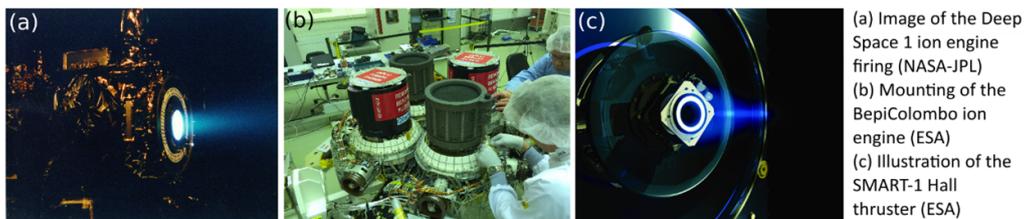


Figure 3. Landmark scientific plasma propulsion missions (GIE = gridded ion engine).

magnetic nozzles and the development of instabilities, remain challenging to study. Predictive models that fully capture such features are yet to be developed but are necessary before high-powered plasma propulsion can be used for manned missions. For physics and engineering, plasma propulsion is proving a fertile field for studying plasma–wall interactions, plume–spacecraft interactions, plasma detachment from magnetic nozzles, electron mobility, plasma oscillations, and performance optimization.

Advances in science and technology to meet challenges

The ever-broadening scope of mission applications for plasma propulsion has driven research and innovation (figure 4), with several key technological issues to be addressed, as detailed above. These outstanding challenges are currently being targeted on four main fronts: technological, simulation, experimental, and theoretical areas [22].

Technological

Several thruster companies have formed in recent years, commercializing innovative ideas advanced by plasma physics researchers through the development of miniature GIEs, electrospray propulsion, alternative propellant technologies, and methods for mass thruster production. Electrodeless systems with increased lifetimes such as the radio frequency (RF) Helicon thruster [23] and the Pocket Rocket plasma thruster have been pioneered by Christine Charles (Australia National University). Progress in EP will include a reduction in the weight and size of power supplies and a wider use of alternate propellants.

Simulations

The development of simulations capturing the physics of thrusters and cathodes is one of the key research areas in plasma propulsion. Numerical simulations (fluid, hybrid, particle-in-cell, and new sparse grid-based techniques) are meant to provide insight into plasma features and behaviour. The key particle-in-cell simulations of Anne Héron (Centre de Physique Théorique, Ecole Polytechnique) [24], the first to definitively show the contribution of azimuthal instabilities to anomalous transport in thrusters, sparked active and targeted research efforts on this topic by several groups worldwide. Community efforts in this area have contributed to recent benchmarking activities [25]. Moving forward, significant efforts are being devoted to the development of 3D codes. Challenges remain, such as the need to simulate high-density thruster plasmas over large domains; methods such as sparse grid techniques are now being applied to accelerate simulations, while still capturing important physics of particle-based codes [26].

Experiments

A new understanding of plasma behaviour is being advanced through experimental tools, for example the optical characterization works of Sabrina Pottinger (Telespazio UK for ESA) and Amelia Greig (University of Texas El Paso), on hollow cathodes and RF thrusters, respectively. Significant work by Sedina Tsikata (ICARE, Centre National de la Recherche Scientifique, CNRS) into laser-based techniques has provided insight into electron properties and the development of plasma waves [27]. The use of physical probes remains standard, and work by Kristina Lemmer (Western Michigan University) has led to marked improvements in the implementation

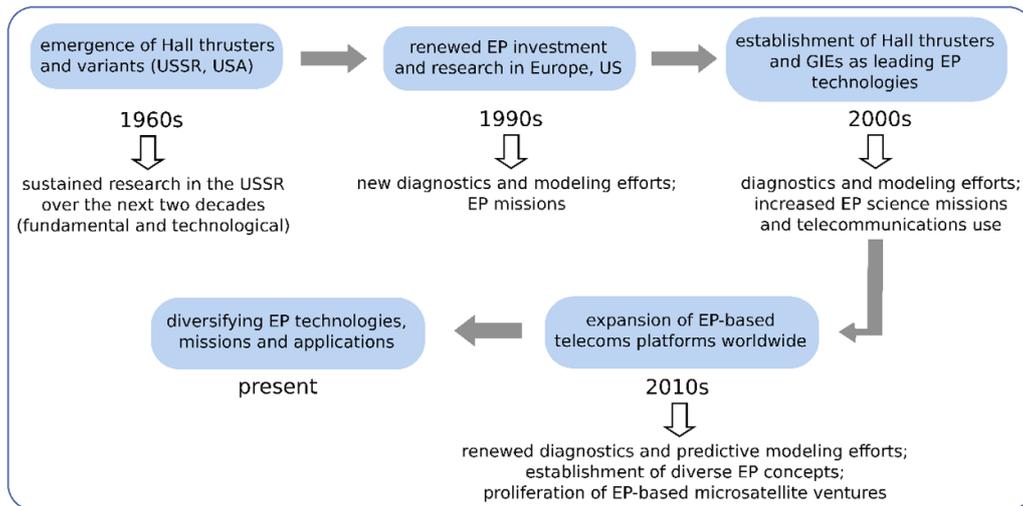


Figure 4. Evolution of electric propulsion over the decades.

of these tools (such as their combination with high-speed electronics and data fusion techniques), thus increasing their capabilities further [28]. The development of additional experimental tools providing access to highly spatially and temporally resolved information is likely to be a key focus in the future.

Theory

Theoretical studies have long sought to describe phenomena linked to macroscopic discharge features [29]. Recent efforts have focused on linear analysis of several types of excited waves, including electron cyclotron drift instability, ion–ion two-stream instability, and modified two-stream instability. While in some cases theory has been updated in response to experimental and numerical observations [30], a significant gap remains to be bridged between theory and a comprehensive understanding of discharge behaviour. Thruster plasmas feature highly non-linear dynamics and theoretical descriptions of many aspects, such as the coupling of different

unstable modes, have remained elusive. Progress in theory will rely on the combination of sophisticated experiments and high-fidelity simulations, still under development.

Concluding remarks

Plasma propulsion systems, since their emergence decades ago, have continued to expand access to space. Such technologies have enabled complex, ambitious space missions, while simultaneously revolutionizing the telecommunications industry by reducing costs and favouring satellite miniaturization. Future progress regarding demanding manned and science missions, new thruster concepts, and operational space challenges hinges on sustained research. Thanks to ongoing efforts in academia, industry, and government worldwide, plasma propulsion remains a truly exciting area of research and innovation. The emerging contributions of women to the advancement of the field is an encouraging development in a traditionally male-dominated area.

3. Super-resolution microscopy

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Status

The resolution of widefield optical microscopy is limited by the wavelength of light and the numerical aperture of the optical system (figure 5(A)). For many years, imaging features separated by less than ~ 250 nm could only be achieved by electron microscopy methods, which do not provide the benefits of targeting and multiplexing for biological contexts. Super-resolution microscopy, a major breakthrough in biological science, overcomes this barrier, enabling fluorescence-based light microscopy to image at resolutions of down to ~ 5 nm or better (reviewed in [31, 32]). Three main approaches have been developed to achieve super-resolution microscopy (figure 5). In structured illumination microscopy (SIM), structured illumination shifts the 'observable region' in reciprocal space to a higher-frequency domain to obtain a \sim two-fold improvement in resolution (figure 5(B)). Stimulated emission depletion microscopy (STED) is a confocal-based technique that uses a depletion laser to switch fluorescence molecules into a dark state (figure 5(C)). The depletion laser has a donut-shaped illumination profile, and is centred around a focused illuminated spot, reducing its size (point-spread function). As the resolution depends on being able to discriminate between two fluorescent spots that are close together, a reduction in their size improves resolution typically by at least four-fold compared to widefield. The final approach (single molecule localization microscopy: SMLM, figure 5(D)) exploits the ability to accurately localize single fluorescent molecules that are well separated spatially, combined with imaging conditions that ensure only a small subset of fluorescent molecules fluoresce at any one time. In an iterative process, subsets of molecules fluoresce and are localized before switching off. Eventually, enough molecules are localized to generate a detailed image with a ~ 10 -fold improvement in resolution compared to widefield. Photoactivated light microscopy (PALM [33]); uses fluorescent proteins, and initially exploited photoactivatable GFP developed by Jennifer Lippincott-Schwartz. Xiaowei Zhuang discovered the photoswitching behaviour of cyanine dyes and developed stochastic optical reconstruction microscopy (STORM [34]).

Since the original descriptions of these techniques, many groups have not only employed them, but developed them further, improving both the physics/optics of these systems, and the analysis of super-resolution images. This is a highly active area of research, with further advances improving both the resolution and usability of this advanced form of imaging.

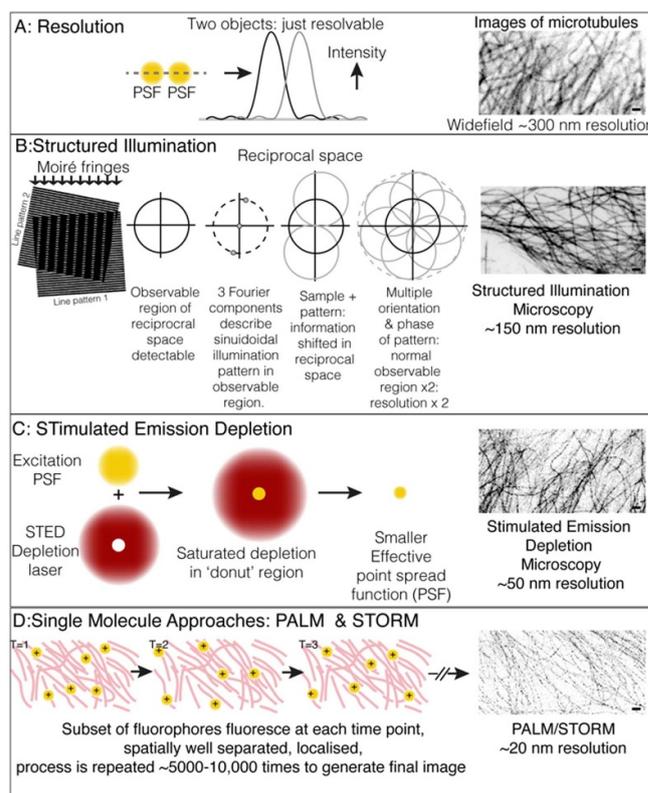


Figure 5. The three main super-resolution techniques. (A) Two fluorophores (shown in yellow) appearing as blurry spots can just be resolved as shown. The point spread function (PSF) for each fluorophore depends on the wavelength of light and the numerical aperture of the optical system. (B) In SIM [35], patterned illumination is used to increase the observable area in reciprocal space, doubling the observable region, and thus doubling the resolution compared to widefield. (C) In STED, a depletion laser is used to deplete fluorophore fluorescence in a donut-shaped region, reducing the size of the effective PSF and thus increasing resolution [36]. (D) In PALM and STORM, only a subset of fluorophores are imaged in each frame, and multiple frames are needed to reconstruct the image. Scale bar $1 \mu\text{m}$.

Current and future challenges

A challenge for super-resolution microscopy is selecting the most appropriate approach [32]. SMLM (PALM or STORM) is commonly chosen as it promises a very high resolution. However, it probably presents the most technical challenges. SMLM relies on software to localize single molecules and to generate the final image, which can be prone to artefacts. Imaging with the expectation of high localization accuracy requires instrumentation that can record images with high precision and localization accuracy (e.g. avoids and/or accounts well for small amounts of drift). Another challenge lies in the choice of fluorescent dyes or fluorescent proteins, with currently a restricted choice as to which work best in terms of photon output at specific emission wavelengths, and in combination for multicolour imaging [37]. Imaging at such high resolutions requires the development of small probes, rather than combinations of large antibodies, avoiding the so-called linkage error. SMLM is one of the slowest approaches,

typically requiring many minutes to acquire enough data to reconstruct an image and needs approaches to increase throughput. There is also the challenge of imaging in live cells, and in small organisms such as bacteria, using SMLM. Interestingly, SMLM has been used for many years to image single molecules in live cells, typically using total internal reflection fluorescence microscopy. The key challenge for sptPALM (single particle tracking PALM) is in choosing a fluorophore best suited for the organism of interest. SIM can be a more straightforward technique as it employs the same fluorophores as those used in widefield and confocal microscopy. Challenges here are to improve the resolution of SIM and reduce potential artefacts in image processing [38]. STED, which has the clear benefit of not requiring any image processing to generate an image, has had to overcome the challenge of imaging speed and of phototoxicity, and challenges in the development of dyes suitable for this methodology. Super-resolution imaging has the additional challenge of being developed for correlative microscopes combined with other types, such as atomic force microscopy (AFM) and cryo-electron microscopy (cryo-EM).

Advances in science and technology to meet challenges

In addressing these challenges, women have played a major role (figure 6). A number of women have worked on developing the software used in SMLM to generate super-resolution images, check for artefacts, and generate artefact-free methods. Susan Cox developed HAWK (Haar wavelet kernel; [39]), which allows discrimination of overlapping localizations in SMLM. Siân Culley has developed NanoJ-SQUIRREL (super-resolution quantitative image rating and reporting of error locations), which compares widefield and super-resolved images to assess SMLM image quality [40]. Melike Lakadamyli has developed methodologies for sptPALM, including the Cega algorithm for tracking particles in live cells [41]. Others have worked on developing the technology. Katharina Gaus developed SMLM technology to improve instrument stability, localization precision and quantification of SMLM images [42]. Na Ji developed adaptive optics to allow for super-resolution imaging of living brains [43]. Sandrine Lévêque-Forte used a combination of shaping the point spread function (PSF) and supercritical angle fluorescence to develop Dual-view Astigmatic Imaging with SAF (supercritical angle fluorescence) Yield, which improves lateral and axial resolutions to 8 and 12 nm respectively and is insensitive to axial drift and sample tilt [44]. Ulrike Endesfelder, Julie Biteen and Jie Xiao all developed methodologies for SMLM imaging in small organisms such as bacteria and archaea [45, 46]. Suliana Manley's group has made many major contributions to the field of super-resolution imaging, including the development of multifocal flat illumination for field-independent imaging illumination for SMLM and instant SIM to both extend the field of view while maintaining a high imaging speed to increase throughput [47]. Ilaria Testa has developed STED methodologies to reduce phototoxicity and increase throughput through the use of RESOLFT (Reversible



Figure 6. Women in super-resolution microscopy: images of the women mentioned in the article, together with the three authors. First row (from left to right): Katharina Gaus (credit: University of New South Wales), Na Ji, Sandrine Lévêque-Fort, Suliana Manley, Xiaowei Zhuang (photos courtesy of the named individuals). Second row (from left to right): Ulrike Endesfelder, Julie Biteen, Jie Xiao, Jennifer Lippincott-Schwartz, Ilaria Testa (photos courtesy of named individuals). Third row: (from left to right): Susan Cox, Siân Culley, Melike Lakadamyli, Marisa Martin-Fernandez (photos courtesy of named individuals). Fourth row: (from left to right): Michelle Peckham, Sang-Hee Shim, Julie Cairney, Lisa Hirvonen (photos courtesy of named individuals).

Saturable Optical Fluorescence Transitions) [48]. In correlative microscopies, Susan Cox and Lisa Hirvonen have developed approaches for correlative atomic force microscopy (AFM) and super-resolution [49], and Marisa Martin-Fernandez has developed correlative cryo-EM and super-resolution microscopies [50] by employing a solid immersion lens to fill the gap between the objective and the sample and increase the effective numerical aperture.

Concluding remarks

Super-resolution microscopy is an exciting, rapidly moving area of research. There continue to be many challenges in improving both hardware and software to capture and analyse images, to improve throughput, to improve imaging in live cells, and to improve dyes and probes. Women have made major contributions to this area of science, and will continue to do so in the future.

4. Bioelectronics

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Status

Bioelectronics looks at the interfacing between biology and electronics, and may bring to mind pacemakers, implantable glucose sensors or deep brain stimulation devices. Since its origins in the 1770s with Galvani, and a later renaissance in the late 1960s, once the origin of ion flow in biological tissues began to be understood, the ability to electrically record and stimulate cells and organs has now become a reality. Bioelectronics is already a fast-moving field and is sure to benefit from parallel advances in personalized medicine and telemedicine, changing the way we access and experience healthcare.

Advances in semiconductor industry and the ability to chemically tune the properties of electronic materials, combined with our ever-increasing understanding of biological systems and processes have resulted in the development of sophisticated bioelectronic devices that can be tailored and targeted as never before. The emergence of nature-inspired electronics, making use of biomimicry as well as natural electronics consisting of living organisms or materials of natural origin, enhance the capabilities of bioelectronics and expand the application scope towards other biological kingdoms such as electronic plants, a field that has been established by Stavriniidou (Linköping University, Sweden) [51]. Energy harvesting devices that harness biochemical reactions in microorganisms are now a reality owing to significant efforts by Boghossian and her team (Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland) [52]. Daniel from Cornell University has been instrumental in expanding the field of bioelectronics all the way from subcellular components such as DNA to cell membranes, for sensing and diagnostics [53]. The era of ‘electroceuticals’ or bioelectronic medicine is upon us, offering tremendous opportunities. Bioelectronic medicine is poised to become a mainstream therapy for a wide variety of conditions ranging from neurodegenerative diseases to inflammatory diseases or even cancer. Bioelectronic devices could be used to treat conditions that today’s drugs and medical procedures are still unable to address, such as severe spinal-cord injuries and blindness. Given the side effects associated with many pharmacological treatments, the idea of an implanted electrical device that can directly stimulate *in situ*, rather than relying on systemic circulation, becomes appealing. Not just implantable, but edible and wearable electronics such as tattoos, and even transient electronics (figure 7(a)), a field where Badhulika and her

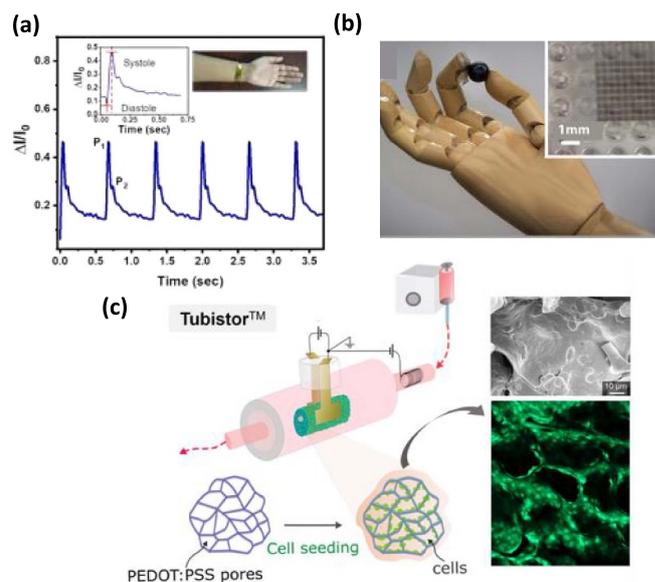


Figure 7. (a) Measurement of radial artery pulse using a wearable, transient nanomembrane-based pressure sensor. Reprinted with permission from [54]. Copyright (2021) American Chemical Society. (b) E-skin image and close-up view on the integrated electrodes. From [56]. Reprinted with permission from AAAS. (c) Schematic of a 3D bioelectronic cell culture device with SEM and confocal images showing cell attachment and growth on a device. From [57]. Reprinted with permission from AAAS.

team’s efforts have been noteworthy (IIT Hyderabad, India) [54], can be envisioned. Bio-inspired information processing is another exciting avenue offering unprecedented capabilities for neuromorphic computing, as shown in a recent study led by Santoro (IIT, Milan) [55], and direct impact in areas such as brain–machine interfaces, prosthetics and robotic skin (figure 7(b)), the latter being established by Z Bao and her team in Stanford University [56].

Current and future challenges

With atomic-scale electronic devices a reality, bioelectronics offer unprecedented opportunities for measuring and manipulating biological matter at different length scales inside or outside the body. However, it is not all plain sailing: electronics have advanced leaps and bounds since the 1960s in terms of speed, capacity and miniaturization, but the things that make electronics suitable for your smartphone may not be the properties that will make them work in your body or with live cells. A large part of current work in the field of bioelectronics is tailoring electronic devices to work more sustainably and efficiently with biological components. Increased synergy between electronics and biology is set to bring a better understanding of biological systems, increase efficiency and effectiveness of medical therapies and yield more sensitive diagnostics. The trend of biological research towards more complex, 3D, multi-cellular, multi-organ systems for more accurate drug discovery needs to be followed by electronics. This means thinking outside the box in terms of device design, e.g. making 3D electrodes interface with 3D

tissues (figure 7(c)), as demonstrated by Owens and her team at Cambridge University [57]. Wearable sensors (including electronic tattoos) provide a whole new range of capabilities for telemedicine when combined with the Internet of Things, but challenges in this space are associated with the device form factor to enable seamless contact with the skin, the processing of raw data, and the need for wireless/low power applications. Implantable bioelectronics have progressed greatly given their promise for precise *in vivo* therapy or monitoring; however most common challenges lie in bio-incompatibility and the need for self-powered operation.

Ultimately, one of the biggest challenges faced by the field of bioelectronics is the translation to the clinic and industry/consumer. This is mainstream in some applications such as pacemakers, cochlear implants and glucose sensors, but these use outdated materials and devices. The new generation of flexible, conformal devices built for purpose are now slowly emerging in clinical trials, a notable example being the work of Lacour and her team at EPFL. A major problem is the approval of new materials for use in medical devices, which will need buy-in from Big Pharma and regulators worldwide. A further issue is one faced by many other fields: that of ethics related to data sharing and privacy. A final, non-negligible issue is related to packaging and electronic waste generation.

Advances in science and technology to meet challenges

The new generation of bioelectronic devices shows huge potential to overcome many of the challenges listed above. In all cases, it is crucial that the devices be designed to fit with biology rather than vice versa. In line with the traditional electronics industry, advances in wireless technology may help solve issues related to device connectivity. Ana Claudia Arias (University of California, Berkeley) has been instrumental in developing devices that require low power consumption, self-powered devices and devices that take advantage of new battery technologies [58]. Examples include energy harvesting from photosynthetic organisms such as plants and bacteria [52]. This is particularly appealing in areas like electronic skin, body-integrated implantable sensors and wearable electronics [54]. For applications such as organs-on-chip and paper-based microfluidics, advances in microfabrication technologies are set to optimize and improve existing geometries, which will help translate these devices from proof-of-concept stage to making them suitable for mass-scale manufacturing.

New generations of electronic materials have now emerged with enhanced material properties establishing effective com-

munication between biology and electronics [55]. Organic electronic materials, for example, are thought of as a synthetically tunable bridge between biology and traditional hard electrodes. When designed for the purpose, they can greatly improve current sensor technologies and open new directions for bio-interfacing, as recently showcased in a pioneering work by Inal and her team (King Abdullah University of Science and Technology (KAUST)) [59]. Moreover they can be chemically tuned to match biological tissue stiffness, and (bio)chemistry, enabling minimally invasive tissue integration. Two-dimensional materials such as graphene or carbon nanotubes [56] exhibit enhanced sensitivity while minimizing device footprint with single molecule resolution for sensing, as shown by Torsi (University of Bari, Italy) owing to the innovative sensor technologies that her team develops [60]. Nanobioelectronics, pioneered by Stevens and co-workers at Imperial College, looks at the biological interfacing at the molecular level through developing high-resolution, micro-/nanoscale architectures while ensuring that device performance attributes including stability, reliability and scalability are not compromised. Last but not least, transient or biodegradable electronics are not only appealing in *in vivo* but are envisaged to address challenges related to electronic waste and environmental pollution. Alongside improvements in integration and bio-interfacing through technological advancements, sensitivity gains in bioelectronic devices are of paramount importance to persuade clinics/labs/industry to take up devices and promote bioelectronic technologies. Also helpful is the fact that bioelectronic measurements can be continuous and label-free [59, 60], which may appeal for clinical translation to allow early detection, increasing buy-in (e.g. more technological pull than push).

Concluding remarks

This is a very exciting time for bioelectronics. Within the next 10 years, we expect to see the routine employment of bioelectronic devices in clinics and diagnostic labs. Bioelectronic devices will work synergistically with traditional pharmaceutical-based approaches, enhancing and targeting therapies. Wearable devices may play a role in preventive medicine, allowing early intervention. We anticipate that the promise shown in initial clinical trials of implanted devices will bear fruit and become widespread in hospitals and surgeries. All of the above will be made possible via a new generation of scientists trained in bioelectronics; we especially note the requirement for creativity in this new field spanning multiple disciplines and embracing people from many geographical locations and of many genders.

5. Spintronics

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Status

The discovery of the giant magnetoresistance (MR) effect, which is said to be the beginning of the spintronics field, has allowed for the increase of the data density of hard disk drives (HDDs) at a rate that exceeds Moore's law, and has contributed to the realization of the current information society. This success in the HDD field has encouraged spintronic researchers to discover many other novel phenomena.

The coupling between spin and transport properties in magnetic materials has allowed access to a non-volatile magnetization state (for storage), an analogous magnetization orientation (for sensing) and a sustained magnetization precession (for oscillating), and use an electrical readout (figure 8). This allowed using the specificity of magnetic materials, in particular their high sensitivity to external magnetic fields, in devices compatible with those of the standard complementary metal oxide semiconductor (CMOS) industry.

A typical spintronic device is a magnetic tunnel junction (MTJ), where two ferromagnetic metallic layers are separated by a thin insulator. Its resistivity changes depending on the relative orientation of the two magnetizations, due to the MR effect. MTJs have been used in all recent HDD heads and open up other applications, e.g. non-volatile magnetic random-access memories (MRAMs), magnetic field sensors, GHz oscillators.

MRAMs are among the candidates to replace Si-based architectures owing to their non-volatility and high endurance. Following the first generation of MRAM using current and magnetic fields to write information, the second-generation using spin transfer torque (STT) was shipped from multiple companies due to higher performance. For example, Tiffany Santos (Western Digital Corp.) *et al* contributed to the reduction of data writing power [61]. In addition, the use of STT for higher output power in nano-oscillators was demonstrated by Alina Deac (Helmholtz-Zentrum Dresden-Rossendorf) *et al* [62], and it has been successfully applied for microwave-assisted magnetic recording in HDD. Later, a comprehensive study of noise control was given by Liliana Buda-Prejbeanu and Ursula Ebels groups (SPINTEC) [63]. In addition, the

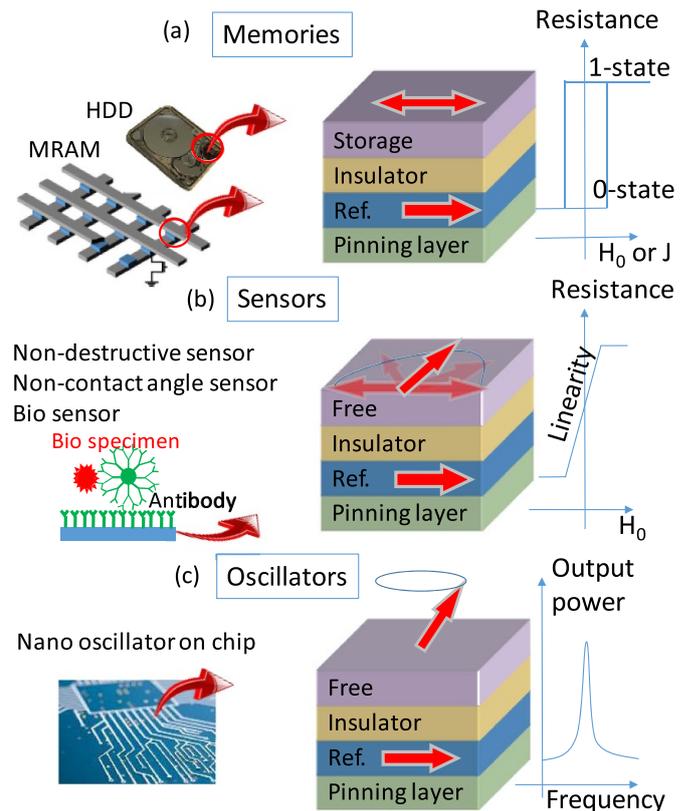


Figure 8. MTJs are used for (a) memories, where the two states are coded by parallel or antiparallel orientations of the storage and reference (called Ref.) layer, for (b) magnetic field sensors where a linear variation of resistance occurs for rotating magnetization of the free layer and for (c) oscillators where sustained precession of magnetization of the free layer leads to output power at a tunable resonance frequency.

phenomena based on spin currents, arising from the difference between up and down spin-polarized currents, have high potential to realize devices without the Joule loss. Spin current can be generated in metallic and insulating magnetic materials from various environmental energies such as heat flows, microwaves, light and even acoustic waves, which can revolutionize the field of spintronics.

Current and future challenges

MTJ with higher MR ratios is demanded for faster MRAMs with lower power consumption. Half metals, with fully polarized density of states at the Fermi level, are good candidates. For instance, Heusler alloys, as proposed by Claudia Felser's group (Max Planck Institute) [64]. In parallel, MTJs have high potential for neuromorphic computing, as reviewed by Julie Grollier (CNRS/Thales), Karin Everschor-Sitte (University of Duisburg-Essen) *et al* [65], as MTJs could perform complex computations with much lower energy costs as compared to conventional CMOS (see also section 14).

To decrease the power consumption of spintronic devices, multiferroic materials have been studied by Agnès Barthélémy's group (CNRS/Thales) [66]. These materials

allow electric fields (instead of charge current) to control their magnetism. The challenge is to find room temperature multiferroic materials with large magnetoelectric coupling and infinite endurance. Charge and spin carrier modulation with electric fields is more efficient in van der Waals magnetic materials, as shown by Jie Shan (Cornell University) *et al* [67]. The difficulties are the low magnetic ordering temperature, limited size, and stability.

Furthermore, current-induced domain wall and skyrmion-based memories are promising as spin torques efficiently move these spin textures. High domain wall-speed in ferrimagnets and magnetic oxide have been shown by Saima Siddiqui (University of Illinois), Caroline Ross (Massachusetts Institute of Technology) *et al* [68].

Further developments for low power skyrmion-based devices use gate control, as shown by the teams led by Anne Bernard-Mantel (Institut Néel, now at Laboratoire de Physique et Chimie des Nano-Objets), H el ene B ea (SPINTEC and Institut Universitaire de France) and Claire Baraduc (SPINTEC) [69]. Challenges are to optimize spin texture velocity, power consumption and reproducibility of their motion for memory or logic applications, and minimize skyrmion size, while keeping stability, in order to support the density of the future memory technologies.

The spin Seebeck effect, a phenomenon originating from spin currents, generates thermopower in a uniform film, allowing energy harvesting. To improve produced power, efficient materials have been proposed by Hiromi Yuasa's group (Kyushu University), for instance [70].

Advances in science and technology to meet challenges

Spintronics technology has already contributed to society, and it will continue to do so in the future. The required performance of spintronic devices in a sustainable society is like that of all other electronics, i.e. ultra-low power consumption, high-speed operation, simplicity of operations and sustainable materials. To realize these features, various spintronic phenomena introduced in the above section have been studied (figure 9) where nano-scaled devices have become standard. Therefore, the improvement of the quality of materials, especially their interfaces, is a critical point to be addressed for many spintronic devices to become more efficient. For instance, spin current-related phenomena often depend on the transmission of spin through interfaces and nontrivial spin textures depends on interface phenomena such as the Dzyaloshinskii–Moriya interaction and perpendicular magnetic anisotropy. Two-dimensional electron gases also greatly depend on interface qualities as they rely on these interfaces to exist. Bulk properties are also of crucial importance to reach optimal spin polarization for improving the MR ratio.

Also, metrology is another challenge to address, in particular for the characterization of very small spin textures such as nanometric skyrmions, very fast mechanisms and very small electrical signals. Synchrotron-based methods (scanning transmission x-ray microscopy, soft x-ray ptychography) and

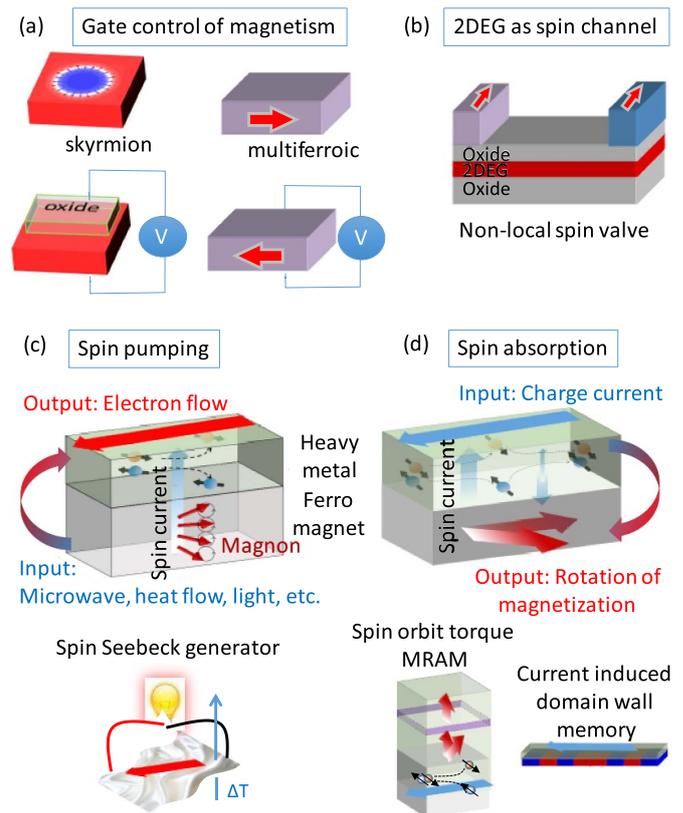


Figure 9. Power reduction and efficiency of spintronic devices may go through (a) gate-controlled magnetism (skyrmions or uniform magnetic state), (b) the use of high mobility 2D electron gases, (c) the use of spin pumping to generate charge currents or (d) the use of spin absorption to control magnetization orientation.

laboratory-level equipment (spin-polarized scanning electron microscopy and high-resolution magneto-optical microscopy) are methods of choice to reach ultimate spatial resolution. Pump-probe experiments allow access to ultrafast mechanisms with the condition of reproducible mechanisms. Electrical characterization of magnetic behaviour is improving, and very small signals are extracted via spintronic-specific approaches, e.g. spin–orbit interactions, spin current, and valley current. Thus, spin is useful not only for the realization of devices but also for the discovery of primitive physics. A combination of all these advantages would be an asset for the full characterization and understanding of spin–orbit-related phenomena and for spintronic device optimization.

In order to use the full potential of spin-related phenomena, one also needs to adapt the device design. Compact models for STT- and spin-orbit torque (SOT)-MRAMs have been or are currently being developed to integrate them as the back-end-of-line in CMOS chips. New designs using the specificity and advantages of spintronic devices are required.

Concluding remarks

Spin interacts with various external inputs and outputs, such as current, voltage, light, heat, microwave, strain, and pressure,

in addition to the external magnetic field. This suggests that spintronic devices may sense these inputs and be operated by them. One of the key factors is the size, and at nanoscales, the contribution from spins becomes apparent. Fortunately, downsizing is the mainstream in microelectronics, so there are many places where spin can play an active role. Domain walls and skyrmions could replace electrons as information carriers and 2D electron gases could be used as channels. Spin-orbit

interactions in nanoscale thin films will help improve MRAM performance. Finally, even if the possibility of MRAMs as the future universal memory is questionable, their optimization either for density or speed should allow bringing non-volatility closer to the processor and even develop in-memory computing. Consequently, spintronics will make a significant contribution to the next generation of the information society.

6. Nanomagnetism

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Status

Nanomagnetism is a very broad field that deals, as the name suggests, with magnetic phenomena on the nanoscale. In particular, both the sample geometry and internal magnetic interactions are highly relevant, yielding diverse magnetic structures and functionalities, which can lead to numerous potential applications.

For example, nanoscale magnetism used in magnetic sensing [71] allows for overcoming limits in magnetic data storage [72], computation and logic, as well as driving innovations in energy harvesting (see section 5). New approaches are pushing forward in biology and biomedicine, such as cell manipulation and separation, particle imaging [73], nano-theragnosis, and nano-magnetic propulsion for minimally invasive surgery.

These targeted end-uses are made possible by the wide range of nanometric sizes and shapes, from zero-dimensional to novel three-dimensional; see figure 10. Most common shapes include nanodisks, nanoparticles, nanowires, and thin films. Through combining different materials, e.g. via thin layer stacking as well as interface engineering, one can further optimize these nanostructures for specific applications. Famous examples include exchange bias in ferromagnetic–antiferromagnetic bilayers, synthetic antiferromagnets, and heavy metal magnetic layered systems to enhance effects such as spin–orbit torques. Furthermore, the interplay of the nanostructures, when arranged in dense arrays, leads to emerging features such as enhanced coupling strengths [74].

Each magnetic sample shape supports different spin structures. The most studied and used ones are single domains, Néel and Bloch domain walls, vortex domain walls, vortices, skyrmions and more recently, magnetic Hopfions. Examples are illustrated in figure 11. Within the last few years, several studies have focused on topological magnetic structures.

Techniques to probe and visualize magnetic configurations where women played a crucial role in their development include spin-polarized microscopy [77] with von Bergmann (University of Hamburg) being a key player in the field, Lorentz microscopy [78], where Yu (RIKEN) has done several pioneering works, and magnetic force microscopy, an area led by Asenjo (Consejo Superior de Investigaciones Científicas—CSIC) and te Velthuis (Argonne National Laboratory), a central figure also in the study of magnetic thin-film structures using neutron scattering. Current requirements are pushing beyond the limits of spatial resolution and detection levels

of standard methods. Recently, highly advanced techniques have revolutionized the field of nanomagnetism, such as x-ray tomography with major contributions from Donnelly (MPI Dresden) [76], electronic and x-ray holography, and nitrogen-vacancy magnetometers with seminal advances by Cappellaro (Massachusetts Institute of Technology) and co-workers [79]. They are bringing the sensitivity and spatial resolution of probing magnetic structures to a new level.

The design of magnetic nanostructures with customized and tailor-made functionalities often resorts to ingenious methods to manipulate magnetic interactions, in particular anisotropy. These include using top-down and bottom-up approaches to nanopatterning, combined with physical and chemical methods to grow and shape the materials [80]. Pivotal and pioneering contributions to develop such new methods include those from Majetich (Carnegie Mellon University), Heydermann (ETH Zurich), and Ross (Massachusetts Institute of Technology). Electron-beam lithography is a widespread and mature technique with proven results in simple and complex device nanostructuring [71, 74] providing a fast track for on-chip integration with electronics [72], photonics, and biomedical technologies [73].

Current and future challenges

With an increasing number of applications in different areas, a central challenge is to control nanostructure design and fabrication. Predicting and uncovering novel functional devices often require modeling their behaviour at multiple length scales, as evidenced by the works of Chubykalo-Fesenko (Consejo Superior de Investigaciones Científicas—CSIC) and Altbir (Universidad de Santiago de Chile—USACH). There is a pressing need for solutions that go beyond micromagnetic simulations, and bridge *ab initio* to atomistic and to submicrometric regimes, while correctly describing magnetic coupling phenomena at the surfaces and interfaces [81]. These become more relevant by potentially incorporating other degrees of freedom such as atomic lattice vibrations (phonons), electrical behaviour, and temperature effects. Such comprehensive simulation tools provide a path for predictive consciousness design of magnetic devices and support the intensified search for alternative or substitute materials. The main goal is to replace rare, expensive, and toxic elements and/or processes, with economical and sustainable solutions.

To fulfil these demands, precise, atomic-level control is necessary for material growth and patterning, side-by-side with high-resolution methods to image and quantify (very small) effects at the nanoscale. The controlled creation, stability, manipulation, and destruction of magnetic structures is essential for realizing next-generation ultra-dense information storage, with reliable operations and high-performance speeds. Recent progress has been demonstrated by Raymenants (Interuniversity Microelectronics Centre) and co-authors [72]. The ability to tune materials with local precision using defects or doping, designing interfaces as well as controllably encapsulating nanostructures, poses a challenge to theoreticians as well as experimentalists. The goals

Geometries in Nanomagnetism

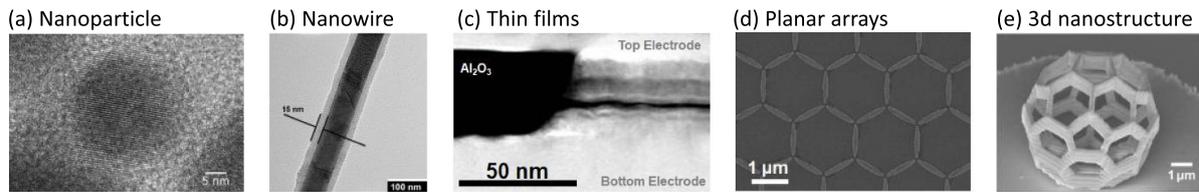


Figure 10. Selection of geometries studied in nanomagnetism: (a) nanoparticle of $Gd_5(Si, Ge)_4$ used in magnetocaloric applications; (b) oxide-shell-protected Mn_5Si_3 nanowire. Reproduced from [75] with permission from the Royal Society of Chemistry. (c) Multi-layered thin-films stack of a MgO-based MTJ used in a nanosensor device. Reproduced from [71]. © IOP Publishing Ltd. All rights reserved. (d) Kagome Ni spin-ice array; (e) co-coated artificial buckyball used for x-ray tomography demonstration. Reprinted (figure) with permission from [76], Copyright (2015) by the American Physical Society.

Spin structures in Nanomagnetism



Figure 11. Selection of spin structures studied in nanomagnetism. [Credit: Sarah Jenkins].

are to develop simple, efficient, yet high-quality, one-step nanofabrication processes [75]. Bottom-up syntheses are viable nano-processes for competitive large-scale production, enabling commercial use. Additionally, direct writing of nanostructures via focused beam techniques, pioneered by Cordoba (Universidad de Valencia), offers a widely versatile route to ‘print’ tailored nanostructures in various dimensions [82].

Beyond fabrication, quality control of the nanostructures is a central responsibility. This involves detecting and probing the electronic, magnetic, and dynamic behaviours of nanostructures. In particular, for medical applications, very high standards need to be met regarding reproducibility, reliability and nano-safety. Thus, for applications beyond magnetism and condensed matter physics, such as medical treatments, interdisciplinary research studies are needed to foster and combine the strengths of the individual research disciplines.

Advances in science and technology to meet challenges

To meet the challenges the nanomagnetism field is facing, advances in all steps, ranging from material research, fabrication processes, characterization, and material quality control, as well as magnetic structure manipulation, are approached by the involved communities.

Improvements regarding the fabrication processes trigger the development of high-quality material growth and advanced nanopatterning techniques. Precise controlled growth of 3D magnetic structures using focused ion and electron beam deposition [82], or template-assisted methods for single or arrays of nanoelements, provide versatile and straightforward 3D packed designs that could be utilized in creating unique

spin-ice structures. Such tailormade 3D structures build the basis for ultra-high-density logic and racetrack memory designs.

Quality control profits from an ever-increasing number of analysis and measurement tools with enhanced signal-to-noise ratios, taking a big step forward in recent years. Fourth- and fifth-generation synchrotrons have higher brightness, better coherence, and incorporate ultra-short pulses (fs), thus allowing us to perform magnetic tomography, holography, angle-resolved photoemission spectroscopy (ARPES), and dynamic probing of single nanosystems. Transmission electron microscopy (TEM)-based techniques, such as spin-polarized microscopy, electronic holography, Lorentz microscopy, are now more accessible for magnetic characterization due to democratization and their widespread use. Additionally, probing of antiferromagnetic structures is now possible because of major instrumentation improvements.

Building new hardware for unconventional computing based on magnetic nanostructures is being explored. Some examples include neuromorphic computing, which is a field that has been founded and pushed forward by the groundbreaking works of Grollier (Université Paris-Saclay) [65], reservoir, stochastic, and edge and memcomputing. Topological objects such as magnetic skyrmions [83] have been put forward as a solution to meet the key challenges of enhanced stability of magnetic nanostructures. Very recent observations of atomic monolayer magnetic materials have made 2D van der Waals magnets a hot topic, with vast unexplored possibilities. The prospect of breakthrough applications also arises from the use of antiferromagnets, which have vanishing stray fields and promising dynamics in the THz regime [84]. Gomonay (Johannes Gutenberg-Universität Mainz) established seminal theoretical foundations in the field of antiferromagnetism.

Growth, patterning, integration, characterization, and manipulation are accompanied by theoretical support, calculations and enormously improving simulation capabilities, enabling bridging different length scales and incorporating more than just the magnetic degrees of freedom. For example, material researchers employ novel composite arrangements, structured analysis techniques and machine learning algorithms to systematically predict new compound materials and magnetic nanostructures. Also, there is a paradigm shift for nanostructure characterization, which typically is performed on few samples and thus lacks statistical information. The rise of big data principles, where thousands of samples are probed in parallel, is anticipated to speed up future research. Similarly, all these building blocks will profit from modern data analysis methods and new machine learning techniques to accelerate progress.

Concluding remarks

The active field of nanomagnetism holds a broad range of applications, the full potential of which has not yet been exhausted. Tailoring high-quality nanomagnetic particles and structures optimally for their individual applications. Additionally, developing innovative functional magnetic materials and properties promises to continue boosting the field beyond magnetism. Each dimension offers different application possibilities and, especially in three dimensions, novel magnetic structures are expected to be discovered about which little is currently known. Combining the knowledge of the involved communities and experimental, theoretical and data scientists, and fostering interdisciplinary research studies, might bring this field to a new level.

7. SQUID technology

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Status

Superconducting quantum interference devices (SQUIDs) combine two physical phenomena—the Josephson tunnelling effect and flux quantization. These devices can measure a tiny change of one flux quantum, Φ_0 , $10^{-6} \Phi_0/\text{Hz}^{-1/2}$, and are the most sensitive detector of magnetic flux demonstrated to date. SQUIDs are classified as low-temperature superconducting (LTS) and high-temperature superconducting (HTS) SQUIDs. LTS SQUIDs are typically made of Nb thin films and Nb/ AlO_x /Nb tri-layer Josephson junctions, operating at the liquid-helium boiling point of 4.2 K. HTS SQUIDs are mostly fabricated from $\text{YB}_2\text{C}_3\text{O}_{7-x}$ (YBCO) thin films using YBCO grain boundaries to form Josephson junctions. They can operate at the liquid-nitrogen boiling point of 77 K. The fundamentals, technology and applications of SQUIDs can be found in The SQUID Handbooks [85]. Although this particular discipline of physics has continually seen a low amount of research, a seminal work to understand dc SQUID noise and its optimization was performed by the eminent researcher, Claudia Tesche, with John Clarke, at University of California Berkeley [86].

SQUID fabrication, cooling technologies, electronics and other system components have undergone significant improvement over the past few decades. SQUIDs today demonstrate more sensitive, effective and reliable operations in applications in biomedicine, standards and metrology, non-destructive evaluation, mineral prospecting and magnetic anomaly detection (MAD) [85]. Due to the page limit, only two areas of state-of-the-art development are briefly reviewed, where women have made significant contributions—biomedicine and geophysics.

In biomedicine, there are two main applications that use SQUIDs (mainly LTS SQUIDs)—the detection of the weak magnetic fields of human body organs (biomagnetism) and the measurement of nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI) signals of spin-1/2 nuclei at ultra-low magnetic field (ULF) strength in the order of tens to hundreds of microtesla (ULF NMR/MRI). After leaving Berkeley, Tesche went on to build her career in biomagnetism by developing the SQUID-based magnetoencephalographic (MEG) methodology for characterizing human brain dynamics at IBM and Aalto University [87].

SQUID-based ULF NMR/MRI benefit from the SQUID's frequency-independent ultra-high sensitivity in the kilohertz or even lower frequency ranges. Compared to high magnetic field MRI, ULF NMR/MRI has the advantage of improved portability, lower cost, enhanced contrast between benign and cancerous tissues, and the possibility of simultaneous

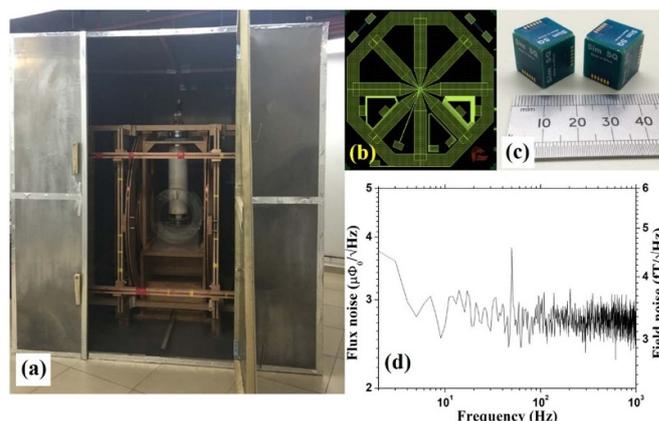


Figure 12. (a) The ULF MRI system developed by Dong *et al* at SIMIT, China. Figures (b)–(d) show the layout, the package and the noise spectrum of LTS SQUID magnetometers fabricated at SIMIT.

acquisition with MEG. Pioneering applications of ULF NMR/MRI have been successfully developed by a number of women, such as a liquid explosive detection technique, a combined MEG and ULF MRI system, by Espy (Los Alamos National Laboratory (LANL)) [88], a dispersion contrast study [89] and magnetic resonance switches for biosensing by Dong (SIMIT) [90], and tumour discrimination by Horng (National Taiwan Normal University) [91]. Figure 12 shows a ULF NMR/MRI system, developed by Dong with her team at SIMIT. The inset figures are the typical layout and noise spectrum of her LTS SQUIDs.

The first application of SQUIDs was in geophysics. The discovery and exploration of mineral ore bodies rely heavily on magnetic measurement techniques. Also, MAD that also uses magnetic measurements is used in military hardware testing, locating large ordnance (e.g. submarines) and environmental surveys such as for landmine detection. For these applications, the sensitivity to low-frequency (0.1 Hz–10 kHz) magnetic fields and gradients is the most important property, and SQUIDs have been used to locate these magnetic sources. A recent review paper by Stolz (Leibniz IPHT) *et al* [92] describes the state-of-the-art development of SQUID-based instruments for geophysical applications including mineral exploration and MAD.

Figure 13 shows an HTS SQUID magnetometer and portable HTS SQUID instruments for mineral exploration (called LANDTEM) and MAD (called UXOMAG), developed at CSIRO. LANDTEM is the most commercially successful SQUID system used for detecting magnetic fields from ore bodies, contributing to the discovery of over \$6B worth of minerals globally, including in Australia. The technology development was led by Cathy Foley [93], with contributions of SQUID development by Jia Du, Emma Mitchell and Jena Lazar (all at CSIRO) [94–98]. Research in this field has inspired and supported many women scientists' careers [98]. This team has been led by women scientists over the last few decades: Foley (1996–2010), Du since 2010 and Mitchell leading another team since 2019. Currently, the team consists of five women scientists who have made many scientific

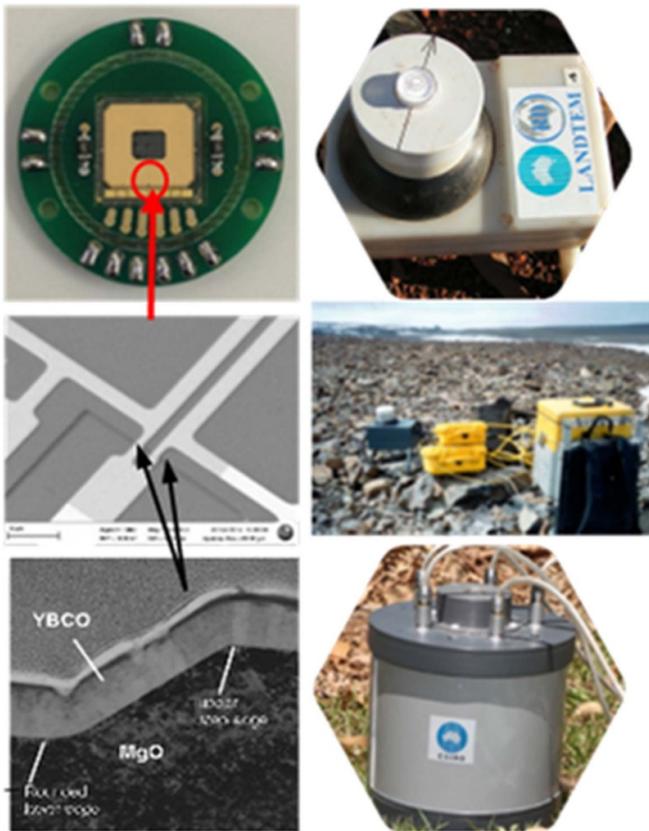


Figure 13. CSIRO HTS SQUID left: an 8 mm pickup-loop dc SQUID magnetometer with close views of the SQUID loop and a TEM image [96] of a step-edge junction and SQUID instruments (right: LANDTEM mineral exploration tool [98] and UXOMAG magnetic tensor gradiometer for MAD) operating in a rugged hostile environment. Reproduced from [96]. © IOP Publishing Ltd. All rights reserved. Adapted from [98], with permission from Springer Nature. Reproduced from [99]. © IOP Publishing Ltd. All rights reserved.

breakthroughs in developing HTS step-edge junctions and SQUID technologies. The team offers a commercial HTS SQUID magnetometer and gradiometer foundry, with a typical field noise of $30 \text{ fT}/\sqrt{\text{Hz}}$ for 8 mm DC SQUIDs and a flux noise of $5\text{--}10 \mu\Phi_0/\sqrt{\text{Hz}}$ for DC SQUIDs of varied designs and sizes with yields over 70%.

Current and future challenges

For sub-fT sensitivity applications required by ULF NMR/MRI, high system noise and environmental interference are major challenges. The intrinsic noise of a SQUID, the noise from the shielding materials inside the dewar vacuum layers and the electrical noise from the power suppliers of the NMR/MRI coils, dominate the system noise. The electromagnetic environment, where the system is placed, can be polluted by, for example, nearby moving magnetic objects and electric power equipment. A direct consequence of high noise is the increase in imaging times required to enable noise reduction by averaging. Slow imaging speed is a key challenge for practical applications of ULF MRI.

The high cost and inconvenience of using liquid helium continues to deter LTS SQUID systems from commercial markets despite their outstanding sensitivities. Helium gas is generally wasted due to it being exhausted. Being an expensive and limited commodity, this means that research on alternative cooling solutions such as compact cryocooling is critical.

HTS SQUID systems offer an obvious practical advantage of a higher operating temperature, and are thus cheaper, smaller and more portable (figure 13). A major challenge for HTS SQUIDs, however, is the difficulty of fabricating cost-efficient, reliable and reproducible Josephson junctions with well-controlled parameters. This is because HTS materials are oxide ceramics and have granular structures, very short superconducting coherence lengths, and are chemically unstable (a propensity to lose oxygen upon exposure to the environment and thus lose their superconducting properties). Painstaking research efforts have been carried out to develop various grain boundary engineered junction technologies and major progress has been made. Nevertheless, improving and maturing HTS junction technology remains a key research topic.

Despite successful examples, commercialization of both LTS and HTS SQUID instruments remains challenging due to their ‘not-so-attractive’ cost-to-value propositions. However, there are some applications that are commercial, such as in mineral exploration.

Advances in science and technology to meet challenges

To overcome the challenge of low signal-to-noise ratios in ULF NMR/MRI, the intrinsic noise of LTS SQUID may be further reduced using a state-of-the-art sub-micrometre junction fabrication technique. Novel materials with minimized metal content are being trialed for shielding materials inside dewars. Artificial intelligence (AI) including deep learning has provided advanced noise suppression techniques, which greatly enhance the signal-to-noise ratio while accelerating the imaging speed. Also, AI techniques potentially provide an effective way to analyse the mass data of ULF MRI images for clinical diagnosis.

Similarly, AI could be applied to geophysical applications (among others) in noise suppression and cancellation techniques, mass data analysis including magnetic source identification and classification and fast imaging or mapping of geological structures.

Advances in cooling technologies are critical for the reduction of the system costs, improved portability, user safety and the convenience required for industrial acceptance. MEG systems are being designed using liquid helium gas circulation to reduce helium consumption and loss. Advances in cryocooler technologies offer the prospect of new ways of cooling SQUIDs instead of using liquid helium or liquid nitrogen. Currently, two-stage cryocoolers (with limited portability) can cool to 4 K, suitable for LTS SQUIDs, and one-stage (portable) cryocoolers can reach 40 K–70 K, suitable for cooling HTS SQUIDs. Further reduction in noise resulting

from vibrational and electromagnetic interference, increase in efficiency in cooling power versus input power conversion and size-weight-cost reduction are required for their future successful application in SQUID systems.

SQUIDs are a relative sensor that only measure fractional changes of the magnetic flux. Research advances developing superconducting quantum interference filters by scaling up to large arrays of SQUID loops will enable absolute magnetic field detection, where sensitivity increases with increasing the number of SQUIDs in the array. Women are leading this frontier research [97, 99].

Without doubt, any advances in new superconducting materials that have higher critical temperatures and/or higher critical currents and critical magnetic fields will make major impacts on SQUID technology by relieving the need for cryogenic cooling and/or improving the device and system performance.

Concluding remarks

Women have been leaders in many aspects of research on SQUID technology, resulting in major contributions to progress in the field over several decades. SQUIDs today are

more sensitive and reliable for many applications. Successful examples include LTS SQUID systems in biomedicine and HTS SQUID systems for mineral prospecting and MAD as described earlier.

Current challenges in SQUID technology include advances in noise suppression techniques, cryocooler technology, device fabrication (including scaling-up to large arrays), new materials and use of AI. If achieved, they will further address the challenges and advance SQUID technology performance, efficiency, reliability, costs and market adoption.

Even though women have played an important role to date, there remains a serious gender imbalance in this sub-discipline of superconducting electronics. We have observed a decline trend in recent years of early- to mid-career women engaged in this research sub-field. Public awareness and organizational efforts are strongly encouraged to tackle this issue. Active actions such as creating flexible working time, offering special scholarships or grants for women returning to research after a period of interruption such as from raising a family and promoting STEM programs would encourage more women students to study physics and superconductivity, and foster greater engagement and leadership opportunities for women scientists.

8. Quantum materials: phenomena and devices driven by symmetry breaking

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Status

Quantum materials are at the forefront of modern physics, exhibiting exotic phenomena related to symmetry, topology, and dimensionality in macroscopic observables. These phenomena can be linked to the Berry curvature of the system, which is a key concept explaining the anomalous behaviour of electrons in a solid [100]. When an electron adiabatically travels in a solid, its wavefunction acquires a phase different from that of an electron in free space. This phase is known as the Berry phase, and the associated gauge field, known as the Berry curvature, changes the equation of motion describing the electron wavepacket. Two resulting effects are the anomalous Hall effect and the spin Hall effect. Furthermore, the quantum anomalous Hall effect and the quantum spin Hall effect can arise in systems where the integral of the Berry curvature over the Brillouin zone, the Chern number, is non-zero. This framework has motivated theoretical and experimental investigation of physical phenomena related to the Berry curvature. A point of particular interest is understanding the impact of symmetry breaking on the Berry curvature and the resulting electron behaviour. Looking at the basic symmetry of the Berry curvature, it has an even function for spatial inversion symmetry and an odd function for time reversal symmetry. Therefore, the Berry curvature becomes zero over all momentum space for a material that maintains both spatial inversion and time reversal symmetries. If time reversal symmetry is broken, the sum of Berry curvatures cannot be zero, leading to the anomalous Hall effect in ferromagnetic materials. On the other hand, if spatial inversion symmetry is broken while maintaining time reversal symmetry, the sum of Berry curvatures over the Brillouin zone is zero. However, the Berry curvature at a specific region in the Brillouin zone can be non-zero, as a result of the dipole moment of the Berry curvature. Berry curvature features prominently in a vast array of materials and devices that fall under the ‘quantum’ category, and the field is rapidly expanding [101, 102]. In this overview, we specifically focus our discussion on three emerging physical phenomena in quantum materials related to the lattice symmetry or the chiral spin structure, which may be understood within the concept of the Berry curvature.

Current and future challenges

One interesting phenomenon is the nonlinear Hall effect introduced by broken inversion symmetry (figure 14(a)). The

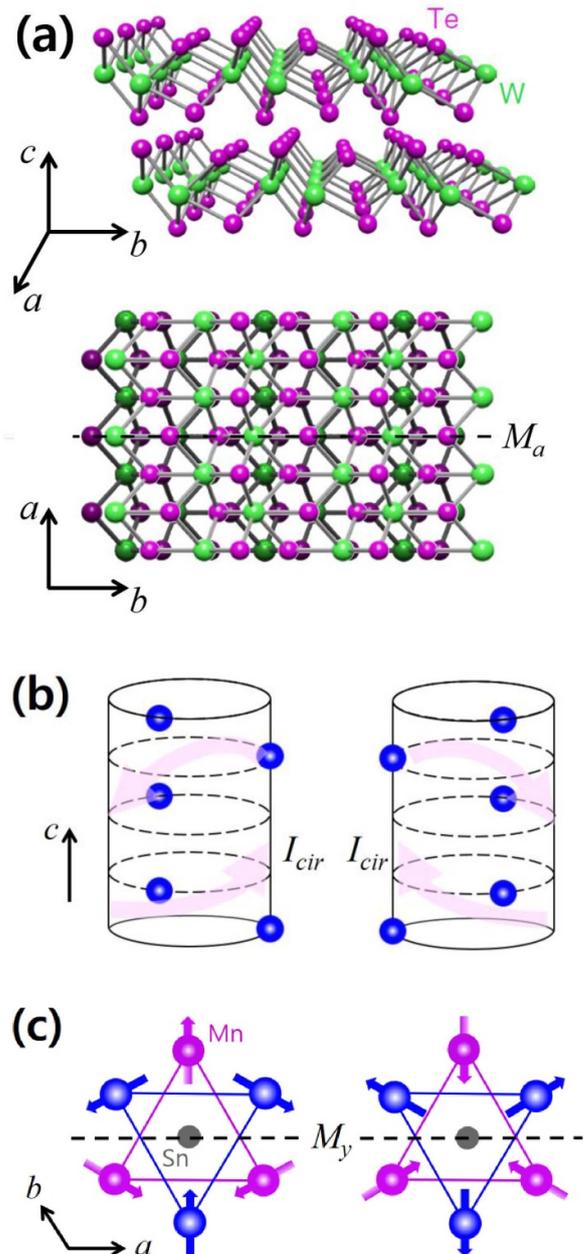


Figure 14. (a) Crystal structure of bilayer WTe₂ with a mirror plane, M_a , where a nonlinear Hall effect is driven by the broken inversion symmetry. (b) Te-type right- and left-handed chiral crystal structures, where an orbital magnetization is expected by applying an electrical current. (c) Crystal structure of Mn₃Sn with a mirror plane, M_y , together with non-collinear right- and left-handed spin configurations, showing an anomalous Hall effect. (e) Allow at most two figures that are roughly the size of this box. If the figure is reproduced or adapted from another non-IOP publication, you must seek permission for re-use from the publisher.

nonlinear Hall effect is the response of a transverse electric field to an applied current parallel to the Berry curvature dipole. Compared to the anomalous Hall effect in ferromagnets with broken time reversal symmetry, the nonlinear Hall effect emerges even in nonmagnetic materials, where only inversion symmetry is broken. For example, Qiong Ma (now at Boston College) and Jie Shan (Cornell University) both

demonstrated that a nonlinear Hall voltage is observed in WTe_2 when an external electric field is applied perpendicular to the mirror plane [103, 104]. However, extrinsic factors such as impurity scattering can generate nonlinear behaviour as well, making it challenging to distinguish the intrinsic nonlinear Hall effect attributed to the Berry curvature dipole. Liuyan Zhao (University of Michigan) has contributed to our understanding of how scattering affects the nonlinear Hall response [105].

A second phenomenon is the emergence of topological quantum properties in chiral crystals (figure 14(b)). The structural chirality in nonmagnetic chiral crystals with spin-orbit coupling leads to a universal topological electronic property due to the lack of crystal symmetry [106]. The topologically chiral fermions, i.e. Kramers–Weyl fermions, that appear at time-reversal-invariant momenta carry nontrivial Chern numbers and act as monopoles or antimonopoles of Berry curvature like conventional Weyl fermions. Recent theoretical results suggest the orbital magnetization is induced by an electric current along the helical crystal axis in the absence of an external magnetic field as a result of broken inversion symmetry [107]. Kyoko Ishizaka (University of Tokyo) has also contributed to the understanding of spin texture in chiral crystals [108].

A third phenomenon of interest is the anomalous Hall effect in non-collinear antiferromagnets (figure 14(c)). The presence of the Berry curvature can enhance the anomalous Hall effect even in antiferromagnetic materials, despite the absence of a net magnetic moment. Examples include Mn_3Ge and Mn_3Sn with a kagome lattice structure [109, 110], where the triangular magnetic order breaks the in-plane hexagonal symmetry of the lattice to induce the anomalous Hall effect. Regarding the non-collinear spin structure, a topological Hall effect is frequently observed in chiral ferromagnetic materials because the scalar spin chirality can generate a fictitious magnetic field, which is also represented as the real-space Berry phase. It may be possible to tune the anomalous Hall effect by controlling the Berry curvature via the symmetry and topological band structure without considering the net magnetic moment.

In order to study the physics of quantum materials, they must first be synthesized. Claudia Felser (Max Planck Institute) has been instrumental in growing a wide range of quantum materials, including WTe_2 and Mn_3Ge [109, 111]. Another universal challenge is to verify if the new phenomena are observed due to the Berry curvature arising from symmetry breaking. Lastly, these newly discovered phenomena have only been intermittently experimentally verified in narrow material groups, making further corroboration and investigation important.

Advances in science and technology to meet challenges

New materials

Access to a wider range of materials with only one symmetry present (inversion or time reversal) can help to elucidate the

role of symmetry breaking as well as expand our knowledge of these phenomena. Leslie Schoop (Princeton University) and Maia Garcia-Vergniory (Max Planck Institute for Chemical Physics of Solids) have advanced the discovery and understanding of a wide range of quantum materials that can aid in this endeavour.

Synthesis

Once we have identified intriguing new materials, we must synthesize them in bulk, film or layer form. Women including Suzanne Stemmer (University of California, Santa Barbara, topological semimetals), Stephanie Law (University of Delaware, topological insulators), Xucun Ma (Tsinghua University, superconductors) and Yanfeng Zhang (Peking University, scalable layered materials) have made significant progress in epitaxy, and these techniques should be extended to newer quantum materials as well.

Measurement

In addition to transport measurements, we can learn about quantum material properties and the impact of the Berry curvature through addition techniques. Women have helped to apply and advance methods for experimentally interrogating quantum materials, including Vidya Madhavan (University of Illinois, scanning tunnelling microscopy (STM)), Ming Yi (Rice University, ARPES), Vivien Zapf (Los Alamos National Laboratory, measurements at high magnetic fields), Shuyun Zhou (Tsinghua University, ultrafast spectroscopies), Lena Kourkoutis (Cornell University, transmission electron microscopy) and Judy Cha (Yale University, measurements of nanostructures). These measurement techniques can be applied to newer classes of quantum materials as they become available. Investigation of interfaces and heterostructures will also be increasingly important, and Adriana Figueroa (Catalan Institute of Nanoscience and Nanotechnology) and others are making progress on this front.

Theory

Theory has helped to direct the quantum materials field in our understanding of both the behaviour of quantum materials and the emergence of new phenomena. Insights into topological and magnetic quantum material properties, such as those provided by Prineha Narang (Harvard University) and Hae-Young Kee (University of Toronto), are needed on the materials development front. Continued progress in computational techniques, such as work by Eun-Ah Kim (Cornell University), will also be important to understand experimentally measured phenomena.

Devices

We are now at the stage of engineering materials with desired symmetries for specific applications. For example, monolayer WTe_2 exhibits the quantum spin Hall effect and electrically tunable superconductivity, while bilayer WTe_2 shows room

temperature vertical ferroelectricity and the nonlinear Nernst effect. A small-angle twist of the bilayer gives rise to unexpected quantum phases such as the giant nonlinear Hall effect, suggesting we may turn the Berry curvature on and off as a function of the twist angle. Furthermore, the nonlinear Hall effect, which is purely an electrical response, offers attractive potential of replacing existing Hall effect devices with non-magnetic materials that do not rely on magnetic fields. Kramers–Weyl fermions in non-magnetic chiral crystals are also useful for a variety of applications, as the chiral charge can induce a real spin texture that is electrically tunable. Likewise, the chiral antiferromagnetic state can be useful for spintronic applications owing to the absence of a stray field that interrupts device selectivity and stability. Finally, it is possible to create hidden quantum phenomena by controlling

the symmetry via artificial methods such as impurity or strain.

Concluding remarks

The discovery of the extraordinary phenomena that arise in quantum materials from the impact of symmetry on Berry curvature has expanded our understanding of condensed matter physics and produced exciting new possibilities for designing devices with novel functionalities. The quantum materials field has only accelerated in the past several years, and it offers unprecedented opportunities for new discoveries and the development of advanced technologies. Women have already made a lasting impact on this field, and the future is bright for early career scientists to make further contributions.

9. 2D materials: synthesis and physical phenomena

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Status

Two-dimensional (2D) layered materials are ultrathin materials possessing relatively high mobility, adjustable energy bands, and topological properties, which can be perfect platforms for fabricating microelectronic devices for the 'post-Moore era' with new technological advances. Among them, semiconducting transition metal dichalcogenides (TMDCs), e.g. MoS₂, have a band gap of 1–2 eV, good air stability and process compatibility for logic integration. To achieve this, the large area uniform growth of TMDC flakes/films with tunable thickness is an essential topic. Chemical vapour deposition (CVD) has been recognized as the most effective route to achieve large-area uniform, large-domain, and thickness-tunable TMDCs with relatively high crystal quality [112, 113]. The fabricated field-effect transistors exhibited high on/off ratios, current densities and mobilities. Women scientists have made significant contributions in this direction. Pengfei Yang and Yanfeng Zhang (Peking University) [112] reported the synthesis of wafer-scale uniform monolayer MoS₂ films with large domain sizes (figures 15(a) and (b)). Very recently, they have also realized the epitaxial growth of wafer-scale single-crystal monolayer MoS₂ vicinal Au(111) thin films, making a significant step towards the large-scale integration of 2D electronics (figures 15(c)–(e)) [114].

Two-dimensional materials have also been the subject of intense research in observing new fundamental phenomena in solid-state systems. For example, 2D TMDCs with a hexagonal crystal structure possess the valley degree of freedom of electrons that are localized at *K* and *K'* valleys in the momentum space (figure 16(a)). Control of the valley degree of freedom by external means is expected to enable the development of novel electronic devices that rely on the manipulation of an electron's quantum degrees of freedom. In this regard, Jie Shan (Cornell University) has shown that circularly polarized light can selectively couple to one of the valleys, allowing the optical initialization of electron's valley index (figure 16(b)) [115]. In addition, Jieun Lee (Seoul National University) has demonstrated the imaging of the valley Hall effect through measuring the valley magnetization generated by an in-plane electric field (figure 16(c)) [116]. More recently, Joolee Son (Seoul National University) reported the strain engineering of a TMDC transistor and showed electrically induced valley magnetization through the generation of the Berry curvature dipole (figure 16(d)) [117].

Current and future challenges

Although great progress has been made in the preparation of 2D materials, their scalable growth still faces huge challenges. The synthesis technologies of wafer-scale, large-domain TMDCs are not yet mature. The dense domain boundaries embedded in the films can greatly hamper the crystal quality and the electrical quality. To increase the domain size of 2D materials, introduction of the element sodium from a soda-lime glass growth template has been confirmed to greatly reduce the growth barrier of monolayer MoS₂ films, enabling the growth of large MoS₂ domains of the size ~400 μm, as revealed by Zhang (Peking University) and her co-workers [112]. In addition, the growth rate of large sized 2D materials is still very low, which is not suitable for industrial-scale production. One method to overcome this problem is to modify the reaction paths by adding catalysts or promoters to reduce the reaction barriers. For example, alkali halides have been demonstrated to effectively promote the growth of TMDCs. Liquid substrates (e.g. molten glass) have also shown unique advantages in the fast growth of 2D materials.

One major challenge in terms of the control of the valley degree of freedom in 2D materials lies in the size of the operating device and its timescale, which are limited by the scattering length and lifetime of the encoded quantum information. The valley lifetime in monolayer TMDCs is known to be limited by the intervalley scattering process mediated through electron–hole exchange interactions. Recently, several efforts to overcome this limitation have been reported, including the fabrication of van der Waals heterostructures composed of different 2D TMDCs (figure 16(e)) [118]. In this approach, electron and hole carriers are separated in different layers, reducing the overlap between the electron–hole wave packet and remarkably extending the valley lifetime and diffusion length. Xiaoqin Li (University of Texas) has also shown observations of interlayer excitons captured in precisely aligned heterostructure moiré potentials, presenting the possibility to explore valley-associated nanophotonics and quantum information technologies (figure 16(f)) [119].

Advances in science and technology to meet challenges

The epitaxial growth of unidirectionally aligned 2D domains has been regarded as a promising route to obtain wafer size single-crystal 2D films. Choosing the epitaxial growth substrate with a good lattice match with 2D materials should hold fundamental significance. Recently, monolayer single-crystal MoS₂ and WS₂ films have been successfully synthesized on Au(111) vicinal facets [120]. Moreover, the transfer process acts as a bridge between the growth and practical application of 2D materials. The polymer residues and etchant damage introduced in the traditional transfer process significantly reduce the crystal quality and electronic performance of 2D

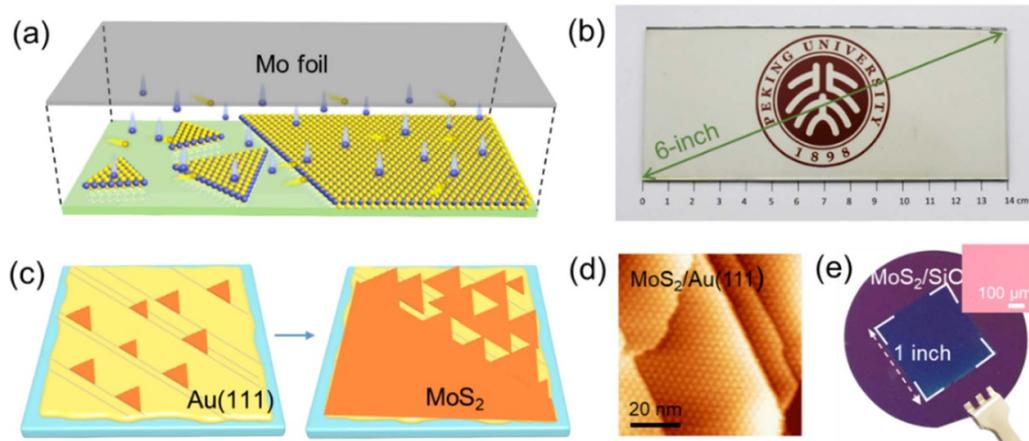


Figure 15. (a) Schematic diagram of a face-to-face metal-precursor supply route for the CVD growth of 6-inch scale uniform monolayer MoS₂. (b) Photograph of a 6-inch continuous MoS₂ film on soda-lime glass. Reproduced from [112]. CC BY 4.0. (c) Schematic illustration of the growth of aligned MoS₂ domains on Au (111) films and their merging into single crystal films. (d) Large-area STM image ($V_{\text{Tip}} = -0.042$ V, $I_{\text{Tip}} = 3.23$ nA) of a continuous MoS₂ monolayer on Au(111). Reprinted with permission from [114]. Copyright (2020) American Chemical Society. (e) Photograph and corresponding optical microscopy image of a 1 inch single-crystal MoS₂ monolayer transferred on a SiO₂/Si wafer. Reprinted with permission from [114]. Copyright (2020) American Chemical Society. Reproduced from [112]. CC BY 4.0.

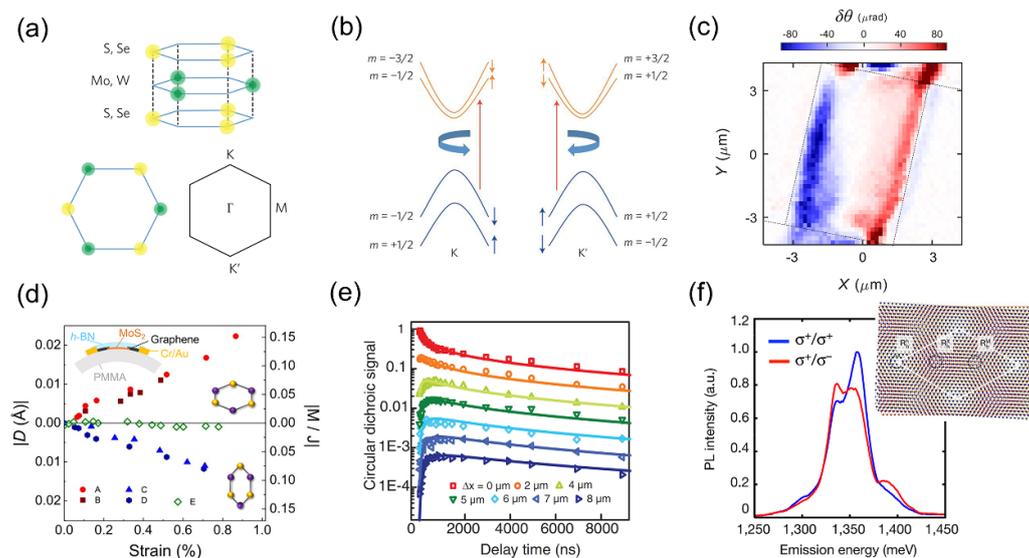


Figure 16. Schematics of the valley degree of freedom (a) and optical selection rule (b) in a 2D hexagonal TMD monolayer. Reproduced from [115], with permission from Springer Nature. (c) Imaging of the valley Hall effect by scanning Kerr rotation microscopy. Reproduced from [116], with permission from Springer Nature. (d) Strain engineering of the valley magnetization per current density (M/J) and Berry curvature dipole (D) in a monolayer TMD. Reprinted (figure) with permission from [117], Copyright (2019) by the American Physical Society. (e) Time- and space-resolved spin-valley diffusion current in a van der Waals heterostructure. From [118]. Reprinted with permission from AAAS. (f) Valley-polarized emission from van der Waals moiré-trapped excitons. Reproduced from [119], with permission from Springer Nature.

materials. On the other hand, layer-by-layer stacking via the sample transfer process is also a versatile way to construct 2D heterostructures and superlattices. However, the clean and sharp interfaces of heterostructures must be maintained to preserve the intrinsic properties of each component and their vertical stacks. Therefore, continuous efforts should be made to develop efficient transfer methods that are environmentally friendly, damage free, and low cost. Transfer strategies using rosin and paraffin as supporting layers have been reported to allow the transfer of flat and clean 2D materials [121].

To observe new phenomena and expand our understanding and perspectives of 2D materials and their applications, the capability to create 2D materials with controlled morphology is a crucial factor. The development of new materials and their characterization will also lead to the observation of novel topological and strongly correlated electron phenomena. Moreover, van der Waals materials and their integration with photonic structures will open up new stages to study light-matter interactions using 2D materials. Developing measurement methods will also enable new observations,

e.g. through novel near-field scanning probe microscopies. By utilizing their high surface-to-volume ratio, 2D materials can also be applicable in classical and quantum sensing devices, as exemplified by Francesca Urban (CNRS). Furthermore, the possibility to realize these interesting phenomena at elevated temperatures will expand the potential applications of 2D materials.

Concluding remarks

Although research on the wafer-scale growth, valley-dependent physics and quantum properties of 2D materials

in the past decade has rapidly developed, it is still in the early stage. To realize the lab-to-fab transition of 2D materials, developing controllable synthesis methods towards wafer-scale, high-quality, single-crystal 2D materials is the first step. By bringing together various quantum degrees of freedom, material properties and tunabilities of 2D crystals and their heterostructures, novel electronics and optoelectronics applications will become available based on 2D quantum devices. We believe that in the next few years more comprehensive progress will be made and women scientists will play pivotal roles in paving the way for discovering new potentials of 2D materials.

10. Catalysis and surface science

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Status

The 2030 United Nations Sustainable Development Goals offer a blueprint for the world to tackle rising CO₂ emissions by transitioning away from fossil resources; if the average global temperature rise is not to exceed 1.5 °C, a large proportion of existing oil, gas and coal reserves must remain unused. Such aspirations necessitate new chemical technologies to produce sustainable transport fuels and value-added chemicals, starting from raw materials such as biomass, CO₂ or water as sustainable feedstocks [122]. The drive for a ‘zero waste economy’ also encourages a circular approach to valorise waste feedstocks. Catalytic materials and an understanding of the fundamental surface science of adsorption processes over catalytic surfaces have underpinned the development of the modern chemical industry, contributing to 90% of chemical manufacturing processes, and facilitating energy-efficient, selective molecular transformations. Many women chemists, physicists and engineers are contributing to groundbreaking research on catalysis, where the design of nanomaterials or photonic materials requires an improved understanding of solid state physics, and the underpinning physics of surface spectroscopies or advanced microscopy and imaging techniques to shed new mechanistic insight into surface transformations over working catalysts [123]. In a post-petroleum era, their efforts will be essential to overcoming the technological barriers to economically feasible processes for low carbon fuels and chemicals production from sustainable feedstocks, including CO₂ capture and utilization. Catalysis at the solid–gas, solid–liquid, or solid–liquid–gas interfaces involves complex surface dynamics that are controlled by adsorption/desorption, diffusion, and speciation, which direct reaction mechanisms and kinetics. The transition to a low carbon society, where chemicals, pharmaceuticals and fuels are produced from sustainable resources, requires new heterogeneous catalysts with nanoengineered active sites and optimized pore networks, guided by *operando* spectroscopy and microscopy [124].

Current and future challenges

Catalysis is a cornerstone of green chemistry, enabling energy- and resource-efficient synthesis of fine and specialty chemicals through selective transformations that minimize by-product and waste formation, eliminate undesirable auxiliaries, and facilitate product separation. The development of low carbon technologies and clean energy through utilization of CO₂ as a chemical feedstock, biomass or water

as a source of carbon and/or hydrogen in order to produce renewable chemicals and advanced transportation fuels necessitates tailored heterogeneous catalysts. Catalysis is also a highly interdisciplinary subject, requiring collaboration at the chemistry–engineering–physics interface. Applied physicists have made significant contributions in several areas including the application of surface science techniques and developing new imaging techniques to understand surface structures and adsorption characteristics of nanomaterials, and the control of electronic properties of photonic materials for photocatalysts employed in solar fuels production from CO₂. Many women of STEM are engaged in advancing materials chemistry and nanoscience, e.g. Rose Amal and Emma Lovell (University of New South Wales (UNSW), Australia), Aiqin Wang (Dalian Institute of Chemical Physics, China), Petra de Jong (Utrecht, Netherlands), Lucia Gorenstin Appel (Instituto Nacional de Tecnologia, Brazil) and Regina Palkovits (RWTH Aachen University, Germany); surface science, e.g. Ulrike Diebold (TU Vienna, Austria) and Cynthia Friend (Harvard, USA); and process engineering, e.g. Laura Torrente Murciano (Cambridge, UK) and Anh Phan (Newcastle University, UK) to accelerate the development of such low carbon technologies. In contrast to fossil-derived crude oil, which has low oxygen content, the high oxygen and water content of biomass-derived feedstocks present challenges for their utilization, requiring innovations in catalyst and process design for the selective conversion of hydrophilic, bulky (macro-)molecules into fuels or high-value chemicals. The design of solid catalysts with tunable porosity will facilitate rapid diffusion of bulky, viscous reactants to active sites; catalyst architectures offering larger pores (compared to zeolites) are thus sought for many processes. The synthesis of hierarchical supports with well-defined, interconnected macro- and mesopore networks, with narrow size distributions tunable over the 100–300 nm and 3–5 nm ranges respectively (figure 17(a)) are particularly effective for enhancing mass transport [125]. The targeted modification of specific functionalities within complex molecules through chemoselective catalysis is also pivotal to achieving a sustainable chemical economy. To this end, selective, multi-step cascade transformations of bio-derived substrates are particularly attractive routes to maximize atom efficiency in chemical synthesis [126]. The rational design of heterogeneous catalysts with optimal performance will rely heavily on a detailed understanding of atomic and molecular interactions and associated reactions at solid surfaces. Advances in the nanoengineering of size-/shape-controlled nanocrystals (figure 17(b)) are required to obtain critical information on the structure sensitivity of molecular transformations, with interrogation by *in situ* and *operando* (under working conditions) spectroscopy, and are key to providing mechanistic insight to guide the design of next-generation catalysts (figure 17(c)) [124]. Leading women researchers including Catherine Louis (Sorbonne University, France), Karine Philippot (Toulouse, France) and Mizuki Tada (Nagoya University, Japan) are advancing the engineering of tailored metal nanoparticles and inorganic catalysts using organometallic precursors.

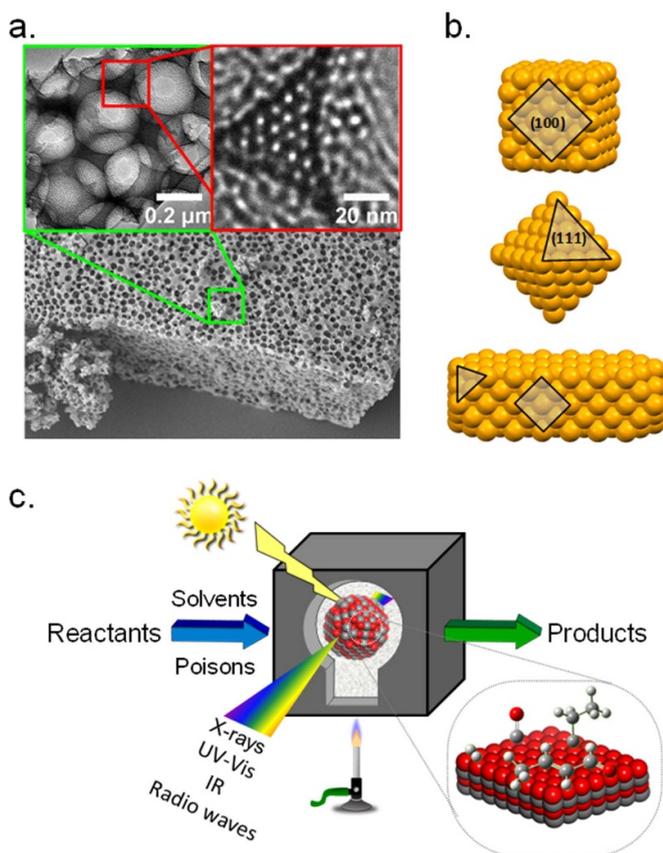


Figure 17. (a) Hierarchical macro-mesoporous networks used to enhance mass transport of bulky reactants; (b) nanoparticles exposing cubic, tetrahedral and bar nanocrystals, preferentially exposing (100) and/or (111) facets to aid structure–activity insight; and (c) *operando* spectroscopy to reveal detailed insight into the nature of catalytic active sites and reaction mechanisms.

Advances in science and technology to meet challenges

Advances in nanoparticle engineering

The design of heterogeneous catalysts by the immobilization of pre-formed colloidal metal nanoparticles can achieve a significantly higher level of control over their nanoparticle constituents' size, shape and composition than traditional impregnation methods. This approach, often termed sol-immobilization (SI), allows nanoparticle properties to be precisely engineered in solution, without interference from a solid phase, prior to their immobilization on the desired support. Work on this has been significantly advanced by the group of Laura Prati (University of Milan). SI is advantageous for achieving monodispersed nanoparticles of uniform composition, and is particularly amenable for designing bimetallic catalysts [127], whether alloys or core–shell structures. However, immobilization of colloidal nanoparticles can be hindered by the organic stabilizing agents that enable their precise engineering. Immobilization can be optimized by a judicious choice of support (e.g. to enhance electrostatic interactions) or by functionalizing their surfaces to improve metal–support interactions (coordination capture).

Nevertheless, stabilizer removal may be necessary to overcome active site-blocking and unlock catalysis, but this process is rarely simple and may not even guarantee better performance. Stabilizer selection is therefore an integral part of nanoparticle engineering. Note that nanoparticle stabilizers can also be beneficial in catalysis, e.g. forming a structured encapsulating shell that can orient reactants, thereby improving product selectivity. However, the stabilizing ligands on metal surfaces may also directly participate in catalysis; N-containing stabilizers activate (previously inert) gold nanoparticles for alkyne hydrogenation [128]. Mechanistic and computational studies indicate this arises from dihydrogen activation via synergy between specific N-containing ligands and the gold surface, which promotes heterolytic H₂ cleavage followed by H⁺ and H[−] pair transfer to alkynes. The ability to induce catalytic activity in otherwise inactive metals offers a promising new strategy to control surface reactivity through ligand design.

Advances in nanoporous materials

Liquid crystal templating is widely used to nanoengineer catalysts with well-defined mesopore networks and an area pioneered by Jackie Ying (A*STAR, Singapore). The Santa Barbara Amorphous (SBA) family of materials generated from block copolymer surfactants (e.g. P123 (PEO₂₀PPO₇₀PEO₂₀)) are particularly attractive due to the wide range of resulting pore diameters (approximately 5–30 nm). However, catalysis of bulky molecules is hindered by slow in-pore diffusion through the long, isolated channels of hexagonal close-packed porous solids such as SBA-15. Dual templating, employing a liquid crystalline mesophase and colloidal polystyrene nanosphere array, yields highly organized hierarchical porous materials (such as MM-SBA-15), whose interconnected and tunable macro- (200–500 nm) and mesopore (5–30 nm) networks can alleviate this issue. Macropores act as high throughput conduits to access active sites within mesopores, conferring striking rate enhancements in the transformation of bulky fatty acids to biodiesel [125].

Strategies to segregate/compartimentalize active sites in 'spatially orthogonal' catalysts are another hot topic in porous materials design due to their potential applications in multi-step organic synthesis. Effective synergy between spatially segregated active sites requires precise control over their location and connectivity to optimize molecular transport, mimicking substrate channelling of chemical intermediates observed in biological systems. Hierarchical porous frameworks (e.g. MM-SBA-15) provide well-defined pathways between active sites, steering reactants from the bulk reaction medium into macropores, with subsequent transport of primary products/reactive intermediates from macropores to mesopores for further transformation. A new strategy to fabricate spatially orthogonal catalysts based on hierarchical porous materials was recently developed, wherein discrete metal or acid–base sites are selectively introduced into macropores or mesopores [129]. Active site compartmentalization and substrate channelling was demonstrated for base catalysed biodiesel synthesis from low quality oils

contaminated with high free fatty acid (FFA) impurity (up to 50 mol%). Rapid esterification within solid acid functionalized macropores neutralised the FFA contaminant, protecting base sites within the mesopores. Routes to spatially orthogonal porous materials and established metallosurfactant templating approaches facilitate the creation of diverse families of dual site catalysts for one-pot selective transformations.

Advances in operando spectroscopy

Molecular insight into catalytic mechanisms often requires surface-sensitive analytical techniques such as diffuse reflectance infrared Fourier transform spectroscopy, sum-frequency generation surface vibrational spectroscopy, STM, or ambient pressure x-ray photoelectron spectroscopy (APXPS). However, meaningful structure–activity relationships also require bridging of the so-called pressure and structure gaps, necessitating analysis under *in situ* or *operando* conditions [130] to identify true active sites and reaction intermediates (versus spectators) and elucidate bonding modes of reactants, intermediates and products, and deactivation pathways under catalytically relevant conditions. Electron paramagnetic resonance, UV–vis and Raman are powerful techniques used to study working catalysts as widely employed by Angelika Bruckner (Leibniz-Institute für Katalyse, Germany). High spatial and temporal resolution of working catalysts has historically necessitated synchrotron spectroscopies to provide such insights via techniques such as x-ray absorption and emission spectroscopies (and their variants) as widely used by Moniek Tromp (Groningen, Netherlands) to study structure/function relationships in homogeneous and heterogeneous catalytic systems, x-ray photoelectron spectroscopy (including APXPS), and x-ray scattering (including pair distribution function (PDF) and resonant inelastic x-ray scattering (RIXS)) to monitor changes in local and long-range chemical composition, structural order and electronic properties [131]. Improvements in synchrotron radiation source flux and pulse mode, detector sensitivity, and the development of x-ray free electron lasers have greatly increased knowledge on the structure and evolution of catalysts under reactive environments, essential for directing the design and manufacture of materials with superior performance, lifetime and reduced operational costs. The structural response of catalysts with reactants not only at the surface but within the bulk of nanoparticles can affect performance (e.g. metal hydride formation). Coherent x-ray diffraction imaging offers insight into the internal deformation field distribution of nanoparticles *in situ* (figure 18) [132], including the localized strain observed at the active sites and the evolution of the defects. Unusual strain evolution related to

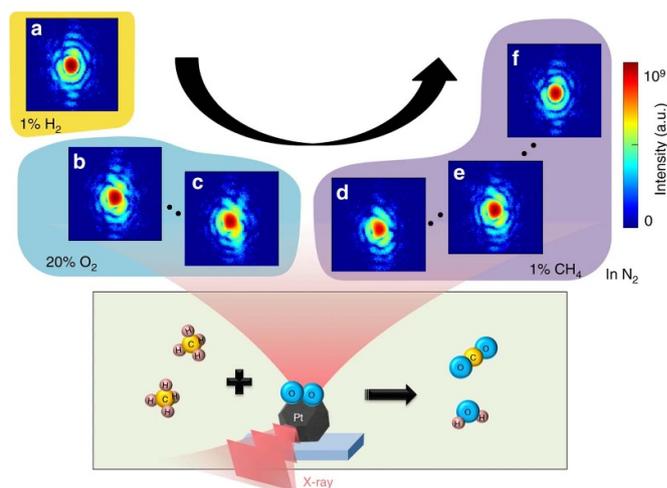


Figure 18. Schematic of *in situ* Bragg coherent x-ray diffraction imaging (BCDI) during methane catalytic oxidation over Pt nanoparticles under different reactive environments. BCDI illustrates the acquisition of (111) Bragg coherent diffraction patterns from the same Pt nanocrystal throughout. After 36 min in H₂ (a); 2.6 min (b) and 36 min (c) after O₂ insertion; ~2.6 min (d), 16 min (e), and 36 min (f) after CH₄ was introduced. Under a 20% O₂ gas flow, the diffraction pattern becomes distorted (b) and (c), and continues to evolve when 1% CH₄ is added before regaining symmetry in (f) owing to completion of the reaction. Reproduced from [132]. CC BY 4.0.

the inhomogeneous organic residue and nonuniform metal ion distribution in nanoporous zeolite crystals has been explored with picometre sensitivity; however, a higher coherent flux is needed to improve spatial resolution to analyse catalytic nanoparticles.

Concluding remarks

Engineering of metal/metal oxide nanoparticles and porous architectures, coupled with molecular insight into their operation through *operando* spectroscopies, has opened new avenues for the rational design of heterogeneous catalysts for sustainable technologies. We envisage a bright future for the development of catalysts for low-temperature atom-economic processes, such as bio-chemo cascades for carbohydrate chemistry wherein immobilized enzymes work in tandem with inorganic nanoparticles in hierarchical porous solids to direct extended multi-step cascades. Realising such aspirations requires development of advanced surface and spectroscopic characterization techniques, offering improved spatiotemporal resolution, sensitivity, and accuracy to address these grand challenges.

11. Opportunities and challenges in development of multivalent batteries

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Status

Lithium-ion batteries (LIBs) are a disruptive technology that has altered the course of human society, making great progress in the last two decades, where their lightweight and high energy density have significantly impacted the portable electronics industry. There have been notable LIB contributions by women battery researchers, such as the European Battery 2030+ initiative coordinated by Edstrom (Uppsala University, Sweden). To ultimately support-grid scale energy storage worldwide, the next generation of high-performance batteries should include alternative chemistries that meet the demands for higher energy density, improved safety and reduced cost, unburdened by a constrained resource supply that limits many LIB technologies. While still emerging, multivalent systems are promising in this regard, as they can potentially lead to higher capacities than monovalent Li^+ ions for storage of the same formula unit of working ions. Herein we discuss some recent contributions from women scientists in the specific arena of ‘beyond Li-ion’ multivalent battery technology. Representative examples of impactful research by women scientists in this field are shown in figure 19.

Current and future challenges

In contrast to weightless electron transfer in semiconductors and electronics, rechargeable batteries are based on a complicated system demanding transport of ions with mass. According to analysis by Rolison (Naval Research Lab, USA) and Nazar (University of Waterloo, Canada), if the annual performance improvement can be expressed as $1/2^n$, where n is the number of transport functions, electron movement in an integrated circuit involves an n of 1, representing a doubling of computing performance every 2 years; for the coupled electron transfer and diffusion of multivalent ions and molecules in a multivalent battery, n is much larger than 3, which predicts less than 10% improvement per year [133]. A specific challenge of multivalent systems is to accommodate the high charge density (M^{x+} , $x \geq 2$), where different types of electrolytes and active materials are needed to achieve effective ion transport.

Advances in science and technology to meet challenges

The alkaline earth metals Mg and Ca are relatively stable compared with Group IA elements such as Li, Na and K

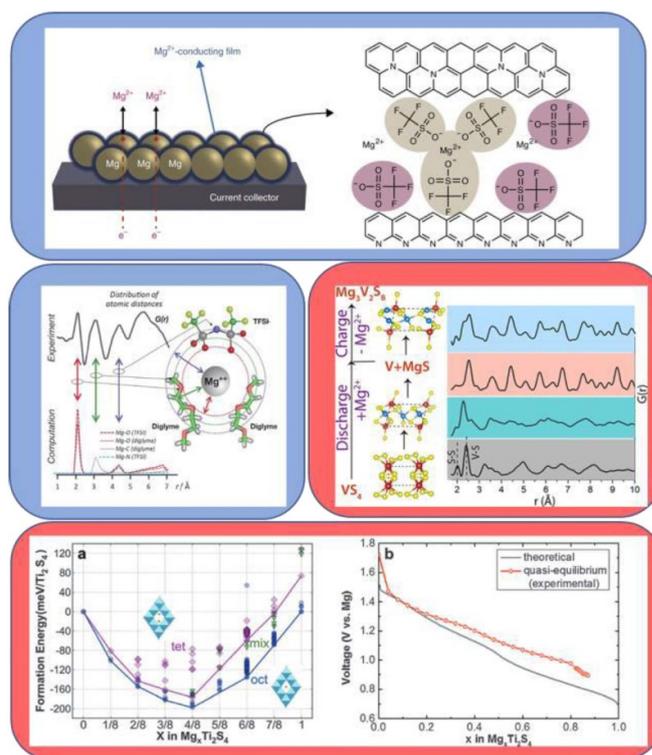


Figure 19. Electrolyte (blue) and cathode material (red) advances in development of multivalent batteries. Reproduced from [139], with permission from Springer Nature. Reproduced from [135]. CC BY 4.0. Reprinted with permission from [146]. Copyright (2018) American Chemical Society. Reproduced from [145] with permission from the Royal Society of Chemistry.

metal; however, they still react with reducible compounds such as carboxylic acids, alcohols, phenols, amines, oxygen, and water. Thus, when used in electrolyte solutions for reversible stripping/plating reactions, oxides and salts (i.e. MgO , MgF_2 , or CaO , CaF_2) form at the surface of metal anodes. To avoid the formation of insulating salts, highly reductive-resistant electrolytes such as Grignard-derived Ph_xMgCl_2 and Ph_yAlCl_3 , magnesium organohaloaluminates were selected [134]. The halogen-based electrolytes stabilize the intermediate partially reduced M^{1+} ions and thus facilitate M^{2+} deposition, as proposed by Rajput (State University of New York at Stony Brook, USA), Persson (Lawrence Berkeley National Lab, USA) and team, as shown in figure 19 [135]. To eliminate the corrosive nature of electrolytes containing halogen ions (Cl^-), Mohtadi (Toyota Research Institute of North America, USA) and co-worker developed $\text{Mg}(\text{BH}_4)$ in glyme, which dramatically enhances the current densities of magnesium deposition [136]. Molecular dynamic simulations combining x-ray scattering data conclude that significantly more contact ion pairs and aggregates are present in multivalent electrolytes than in their monovalent counterparts, and suggest weakly coordinating anions leads to little or no ion pairing that better support the Mg electrode position [137]. As recently reported by reported Mohtadi, Yao and co-workers, using a boron cluster-based weakly coordinating electrolyte facilitates fast Mg^{2+} migration but also enables dendrite-free Mg

plating/stripping at a current density of 20 mA cm^{-2} [138]. In parallel to electrolyte development, interphase engineering has been proposed as another strategy by Ban (University of Colorado Boulder, USA) and co-workers to enhance reversible Mg chemistry through design of artificial solid-electrolyte interphase, enabling reversible Mg stripping/plating not only in Grignard-based electrolytes but also in water-contained carbonate-based electrolytes [139]. The feasibility of using anatase-phase TiO_2 as an electrode material for Mg ions was studied by Meng (University of Chicago, Chicago, IL; Argonne National Lab, Lemont, IL, USA) and co-workers, who illustrated using spectroscopic and microscopic techniques that a Mg:Ti ratio of $\sim 0.1:1$ could be inserted electrochemically or chemically without phase transformation [140].

Ca stripping/plating was firstly reported with $\text{Ca}(\text{BF}_4)_2$ -containing electrolyte at an elevated temperature (100°C) by Palacín (Institut de Ciència de Materials de Barcelona, Spain) *et al* [141]. Later, reversible Ca electrochemistry was realized at room temperature using a borate salt with an anodic stability of $4.1 \text{ V vs Ca/Ca}^{2+}$ [142]. However, the deposition of insulating CaF_2 was observed in both electrolyte systems, resulting in low Coulombic efficiency. Inspired by the development methodology for Mg electrolytes, a boron-based Ca electrolyte $\text{Ca}[\text{B}(\text{hfp})_4]_2$ in dimethoxyethane (DME) was developed to reach an oxidative stability $\sim 4.5 \text{ V}$, albeit with a reduced amount of CaF codeposition [143].

Improvements in electrolytes for Mg have accelerated the development of intercalation cathodes for multivalent batteries. An ideal magnesium cathode can accommodate reversible intercalation or conversion along with insertion/release of one magnesium ion per cathode formula, thus offering the promise of nearly double the capacity offered by existing LIB cathodes. Marschilok (State University of New York at Stony Brook and Brookhaven National Lab, USA), Takeuchi (State University of New York at Stony Brook and Brookhaven National Lab, USA) and team reported an enhanced reversibility of Mg (de)intercalation by using hydrated V_2O_5 xerogels due to water content and porous structures for more surface diffusion [144]. Nazar's group demonstrated promising electrochemical performance for the spinel $\text{Mg}_x\text{Ti}_2\text{S}_4$ with a capacity approaching 80% of the theoretical (239 mAh g^{-1}) [145]. First-principles calculations predicted low diffusion barriers in the calcium ferrite-type post-spinel structures; however, it has

been challenging to stabilize these materials during synthesis, as shown in figure 19 [146].

Different from intercalation cathodes, materials that undergo a conversion reaction with multivalent ions can accommodate more than one multivalent atom per formula, thus leading to higher theoretical capacities. With sulfur as a cathode, a Mg–S battery yields a theoretical specific energy of 1722 Wh kg^{-1} . When using a non-nucleophilic Mg $[\text{B}(\text{fip})_4]_2$ (fip is $\text{OC}(\text{H})(\text{CF}_3)$) electrolyte, Zhao-Karger (Helmholtz Institute Ulm, Germany) *et al* demonstrated excellent long-term Mg cycling stability with a capacity of 800 mAh g^{-1} and high anodic stability of $\sim 4.5 \text{ V}$ [147]. Recent investigations by Grey (University of Cambridge, England) *et al* through multi-scale characterization techniques confirmed an alternative conversion cathode based on transitional metal polychalcogenide containing discrete $[\text{S}_2]^{2-}$ bonds (such as $\text{FeS}_2 \text{ VS}_4$) [148]. Results indicate that the structural transformation of VS_4 follows a combined cation–anion redox-mediated process through a formation of an intermediate phase ($\text{Mg}_3\text{V}_2\text{S}_8$) followed by a conversion reaction to the final products of the V metal and MgS. Thus, with both cations and anions involvements in conversion reactions during multivalent insertion–deinsertion, a VS_4 cathode can deliver a capacity of 250 mAh g^{-1} .

Concluding remarks

Rechargeable batteries are ubiquitous in our daily life and significantly impact the future development of electronic devices, electric vehicles, and renewable energy. Despite the huge success of LIBs, there is a strong incentive to explore other electrochemistry to increase energy and power densities with reduced cost. This section discusses recent contributions from women scientists in the specific multivalent systems to be addressed. While it is not possible to comprehensively describe all significant research in this important area in this format, our goal has been to celebrate the contributions of women in science to multivalent batteries with studies focusing on interface stability, Mg^{2+} intercalation chemistry in cathodes and the development of Mg^{2+} electrolytes. Ultimately, our hope is to inspire the next generation of women scientists and engineers to continue the development of beyond-lithium-ion technologies in their own work.

12. Fuel cells

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Status

Fuel cells operate in one of two general temperature regimes: around 80 °C or above 600 °C (figure 20). Polymer electrolyte fuel cells (PEFCs) are low-temperature energy-conversion devices that are used in transportation and stationary power applications. Their advantages include dynamic response, fast start-up/shut-down, high-power densities and zero-emissions [149]. Low-temperature fuel cells, originally developed for space applications, have found other markets, being broadly deployed in residential power (ENEFARM) and transportation, in which most major automakers (Toyota, Nissan, Hyundai, Honda, BMW, GM, etc) have released or plan to release fuel cell cars. Most recently, PEFCs have entered the heavy-duty truck market, where their high specific energy, short refuelling time and long-driving ranges make them very competitive. Cost and durability are major hurdles to be overcome for broad commercialization of PEFCs. On the other side of the spectrum, high-temperature operating fuel cells include molten carbonate fuel cells (MCFC) and solid oxide fuel cells (SOFCs). MCFC technology has been deployed for large-capacity power plants for decades by companies such as Fuel-Cell Energy. SOFCs are based on oxide ion-conducting materials and have been intensively researched both in academia and industry. Conventional SOFCs operate at the highest temperature regime (≥ 700 °C). This characteristic high-temperature operation provides numerous advantages, especially for stationary applications. For example, an SOFC has the highest efficiency and specific energy in comparison with other fuel cells and is capable of using fuels other than pure hydrogen (fuel flexibility) by much simpler reforming than that of low-temperature fuel cells.

Numerous women pioneers have contributed to the advancement of both PEFCs and SOFCs. Scientists such as Debbie Myers (Argonne National Laboratory), Shanna Knights (Ballard Power Systems), Renate Hiesgen, Karren More (Oak Ridge National Laboratory), Deborah Jones (University of Montpellier), Laure Guétaz (University Grenoble Alpes; CEA, LITEN), Sylvie Escribano (University Grenoble Alpes; CEA, LITEN), Aimey Bazylak (University of Toronto), Perla Balbuena (Texas A&M University), Anna Stefanopoulou (University of Michigan), Signe Kjelstrup

(Norwegian University of Science and Technology), Svitlana Pylypenko (Colorado School of Mines), Christina Johnston (Bosch), Mehtap Oezaslan (TU Braunschweig), Laetitia Dubau (University Grenoble Alpes; CNRS, LEPMI), Jia Wang (Brookhaven National Laboratory), Tatiana Reshchenko (Hawaii Natural Energy Institute), Sara Cavaliere (University of Montpellier), Monica Dutta (Ballard Power Systems), Julie Bellerive (Ballard Power Systems), Huyen Dinh (National Renewable Energy Laboratory), Christina Roth (University of Bayreuth) and Hongmei Yu (Chinese Academy of Sciences) have played a critical role in supporting PEFC advancements from research to commercialization. Ellen Ivers-Tiffée (Karlsruhe Institute of Technology), Rotraut Merkle (Max Planck Institute), Anke Hagen (Technical University of Denmark), Sossina Haile (Northwestern University), Bilge Yildiz (Massachusetts Institute of Technology), Olga Marina (Pacific Northwest National Laboratory), Jennifer Rupp (Massachusetts Institute of Technology), Nicola Perry (University of Illinois at Urbana-Champaign), Min-Fang Han (Tsinghua University), Pei-Chen Su (Nanyang Technological University) are some of those who have significantly contributed to fundamental and application aspects of SOFCs. Pictures of selected women pioneers are shown in figure 21.

Current and future challenges

Within the PEFC stack, the electrocatalyst cost does not benefit from economies of scale and constitutes 31% at 500 K systems/year. For fuel cell vehicles to meet cost parity with internal combustion vehicles at $\$30 \text{ kW}^{-1}$, overall electrocatalyst (Pt or Pt-alloy) use in PEFC stacks must be reduced. Pt is a critical component of the PEFC stack, as it catalyses the sluggish oxygen reduction reaction. Typically, nanoparticles of Pt are supported on carbon and bound by ionomers into a 5–10 μm thick catalyst layer. Reduction of Pt loading in the PEFCs is a challenge, as both efficiency and durability of the stack will be affected. A current challenge is to achieve higher PEFC efficiencies by operating at higher temperatures (> 100 °C). However, polymer membrane and ionomer stability at these higher temperatures is highly demanding. Renate Hiesgen, a dedicated fuel cell scientist who is no longer with us, was one of the first to suggest that ionomers should not be overlooked and showed ionomer degradation in catalyst layers with AFM [150]. PEFC deployment also faces challenges due to competitive battery technologies. Shanna Knights has made major contributions to PEFC commercialization in buses at Ballard Power Systems with more than 25 years of experience, focusing on understanding durability [151].

To raise the maturity of SOFC technology to commercialization, intensive efforts are still ongoing to overcome the hurdles of reliability. Although high-temperature operation provides distinctive merits to SOFCs, it often seriously deteriorates their longevity. Women pioneers have been dedicated to challenging these issues by understanding the fundamentals and thus to improve the durability of SOFCs. Ellen Ivers-Tiffée has elucidated the electrical/electrochemical reactions and transport processes at

Fuel	Anode (Oxidation of Fuel)	Fuel Cell Type: Electrolyte (Operating Temperature) Conducting Ion	Cathode (Reduction of Oxidant)	Oxidant
Internal reforming $H_2, CO \rightarrow$	← H_2O CO_2	SOFC: Solid Oxide ($\geq 700\text{ }^\circ\text{C}$) ← O^{2-}		← O_2 (air)
Internal reforming $H_2, CO \rightarrow$	← H_2O CO_2	MCFC: Molten Carbonate ($650\text{ }^\circ\text{C}$) ← CO_3^{2-}		← O_2 (air) CO_2
External reforming $H_2 \rightarrow$		PAFC: Phosphoric Acid ($250\text{ }^\circ\text{C}$) $H^+ \rightarrow$	→ H_2O	← O_2 (air)
Internal reforming H_2 (CO removal) →		PEMFC: Polymer ($80\text{ }^\circ\text{C}$) $H^+ \rightarrow$	→ H_2O	← O_2 (air)
H_2	← H_2O	AFC: Polymer ($70\text{ }^\circ\text{C}$) ← OH^-		← O_2 (air) (CO_2 removal)

Figure 20. Summary of fuel cell types and operation. Reproduced from [158], with permission from Springer Nature.

the surfaces and interfaces of SOFCs, and Rotraut Merkle has contributed to a profound understanding of proton-conducting (protonic) ceramics. Bilge Yildiz has illuminated reaction and transport kinetics of SOFC, especially at the surface, with her expertise in scanning tunnelling microscopes, and Olga Marina has developed advanced SOFC materials and is dedicated to understanding degradation mechanisms. Anke Hagen and Min-Fang Han have pioneered wide spectrum of SOFC R&D, covering materials to systems.

Advances in science and technology to meet challenges

To address PEFC durability, understanding of the catalyst degradation processes is needed. Deborah Myers has pioneered *in situ* and *operando* synchrotron x-ray techniques to probe electrocatalyst dissolution under fuel cell operating conditions [152]. X-ray scattering analysis showed Pt particle growth with the number of cycles, indicating continuous loss of active surface area. One strategy to mitigate Pt particle growth is to anchor particles onto supports to reduce dissolution or agglomeration. Shanna Knights has worked with other researchers to develop nitrogen-doped supports and showed that with increase in nitrogen content, Pt particle growth is reduced. The observation of catalyst, support and ionomer distribution is challenging, and Karren More, Laure Guétaz and Sylvie Escribano have spent years developing TEM tools for visualizing PEFCs components. These tools have helped the field advance the understanding of morphological transformation during ageing. Their latest achievement is ability to image ultrathin Nafion layers within catalyst layers

[153]. Deborah Jones has led several major fuel cell projects in Europe to enable higher-temperature operation of PEFCs through the design of novel membranes with high performance and durability [154].

Durability is also a challenge on the high-temperature side. Fuels, oxidants, steam, and electrochemical reactions at high temperatures often induce unwanted chemical reactions, which leads to fast SOFC degradation. Consequently, achieving lower operating temperatures ($T_{\text{operation}} \leq 600\text{ }^\circ\text{C}$) without compromising advantages such as higher cell efficiency and fuel flexibility has been one of the most important challenges of SOFCs. There have been two major approaches to reduce the operation temperature of SOFCs. One is to use novel materials with superior electrical and electrochemical properties, and the other is to minimize cell resistances by using thin films and nanostructures. Sossina Haile has reported remarkable achievements both in performance and stability of a protonic ceramic fuel cell with advanced materials. A peak power density of 0.548 W cm^{-2} at $500\text{ }^\circ\text{C}$ and long-term stability under CO_2 were reported [155]. Pei-Chen Su first reported three-dimensional ultra-thin SOFC free-standing membranes [156], which initiated innovative research activities on unprecedented low-temperature SOFC performance with 3D structures. Nevertheless, the mechanical frailty of the free-standing membrane induces fatal problems in stability. To overcome this issue, a combination of the conventional ceramic platform and thin film technology has been developed at the Korea Institute of Science and Technology, called multiscale-architected LT-SOFCs. Both high performance and long-term stability are secured, and recently peak power density of over 0.65 W cm^{-2} at $500\text{ }^\circ\text{C}$ with exceptional redox cycle stability was reported [157].



Figure 21. Selected women who have contributed to PEFC research, development and deployment. First row (from left to right): Deborah Myers (Credit: Argonne National Laboratory), Shanna Knights, Karren More (photos courtesy of the named individuals). Second row (from left to right): Perla Balbuena, Anna Stefanopoulou, Renate Hiesgen, Sylvie Escribano (photos courtesy of the named individuals). Selected women who have contributed to SOFC research, development and deployment. Third row (from left to right): Ellen Ivers-Tiffée, Rotraut Merkle, Anke Hagen, Sossina Haile (photos courtesy of the named individuals). Fourth row (from left to right): Bilge Yildiz, Olga Marina, Min-Fang Han, Pei-Chen Su (photos courtesy of the named individuals).

Concluding remarks

The last decade has seen much advancement in low-temperature fuel cell development and deployment. PEFCs will see broad deployment in heavy-duty transportation and residential power. Currently, cost and durability are still challenges that need to be overcome. Women scientists and engineers have significantly advanced both the technology and

commercialization of PEFCs. Likewise, significant advances in SOFC science and technologies have been achieved by numerous pioneering women researchers. Lowering the operating temperature without compromising performance is one of the topics that women pioneers have challenged and contributed to substantially. There are now many more women researchers in the fuel cell field, especially in the last several years. They will become leaders in the field in the next decade.

13. A brief her-story of photovoltaics (PV)

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Status

Solar PV, the conversion of light into electricity, is versatile, cost-effective and is now the fastest growing form of electricity generation, such that the International Energy Agency (IEA) anticipates that PV will be the dominant source of electricity by 2050 in a growing market for energy [159]. As a renewable and distributed electricity generation solution, PV has inspired generations of motivated women to contribute to PV development in laboratories, factories, education and field deployment using science and technology, as well as policy and social acceptance.

While the PV effect was first observed in the 1830s [160], it took until the 1950s to demonstrate the first working silicon cells [161]. The technology gained traction in the 1970s with growing interest in powering space exploration and when the oil crisis drove public and political interest in energy independence.

The USA took an early leadership position in R&D and women started to gain a profile for their contributions. Terry Jester (SolPad) started with Arco Solar in 1979, working on module design to improve reliability and has been an industry mainstay. Sheila Bailey (NASA), a senior physicist, worked on space PV at NASA for 33 years, and Sarah Kurtz (UCMerced) started working on multi-junction solar cells (GaInP/GaAs) in the mid-1980s, moving to reliability and, more recently, the challenges of solar integration at terrawatt (TW) scale. Sarah was recognized in 2012 for a lifetime of achievement with the William Cherry Award.

The USA continued to contribute to solar R&D, making significant contributions in thin-film materials development, module reliability and financing. Manufacturing of now-dominant silicon technology, however, moved with the markets. First Japan offered incentives in the 1990s, creating a demand for solar, followed by Europe, in particular Germany, resulting in substantial technology advancement, including improvements in efficiency and market development. Francesca Ferrazza (ENI), led one of the early research programs in Europe on Al-back-surface field improvements and manufacturing, and Mechthild Rothe (Becquerel Prize, 2008) developed energy policy that motivated investment in PV. Nicola Pearsall (University of Northumbria) was an early pioneer in many fields of PV technology including solar cells for space, building integrated PV, and PV system performance. Martha Lux-Steiner (Helmholtz Zentrum Berlin) contributed significant work in the fundamental physics and development of materials systems and thin-film devices.

Silicon supply was seen as a potential barrier to growth in the early 2000s. In response, a number of thin-film technologies emerged as contenders for low-cost, high volume PV. Ingrid Repins (NREL) led US development of CZTS and reliability of CIGS. Ilka Luck (Heraeus Start-Up) was a founding partner of Sulfur Cell in Germany.

Throughout this early market development stage, researchers continued to make improvements to the fundamentals of solar cell technologies, with new benchmarks set and broken every year—driving development and motivating improvements in manufacturing.

The researchers active in this highly competitive environment were set to play a significant role in the next stage of PV technology development. Aihua Wang (China Sunergy) played a leading role in many of the high-efficiency records set at UNSW, Sydney, before going on to be a co-founder and CTO of China Sunergy, one of the early solar module manufacturers in China. Wang was soon followed by others, with Ximing Dai (Alex Solar), also of UNSW, co-founding JA Solar, and Cindy Hu (Yingli) becoming R&D director of Yingli, one of the first PV giants.

Incredible progress continues to be made, with women playing key roles. Technology improvements and economies of scale continue to drive down costs with large-scale manufacturing achieved in China (see figure 22). Madam Mi (SNEC) established and runs SNEC—the world's largest solar PV technology showcase. In the USA, Lidija Sekaric (Sun-Run) and Becca Jones Albertus (US Department of Energy) implemented the Sunshot initiative, working towards the goal of $\$0.06 \text{ kWh}^{-1}$. In Australia, Renate Egan (UNSW) co-founded Solar Analytics and now leads UNSW research activities at the Australian Centre for Advanced PV. In research and education, Christiana Honsberg (Arizona State University and winner of the Cherry Award, 2015), Jenny Nelson (Imperial College London) and Anna Bruce (UNSW) have built on their early technology contributions to establish leading programs in PV and integration.

Importantly, tracking the phenomenal growth in PV, with a technology and market lens, Paula Mints (SPV Market Research), Jenny Chase (Bloomberg NEF) and Izumi Kaizuka (RTS Corporation and winner of the 2017 PVSEC Special Award), and Lv Fang (Chinese Academy of Sciences) have provided market research information, tracking markets, innovations and improvements in the technology.

Current and future challenges

Solar is now the lowest-cost form of electricity generation. It is both disruptive and still an emergent technology. In the last 4 years, the industry has shifted to a cell technology known as mono-PERC. This technology, based on p-type monocrystalline silicon, has a potential conversion efficiency estimated to be around 24% commercially [163]. Champion module efficiencies (figure 23) continue to increase for all cell technologies with single-junction c-Si now over 24%. Coupled to the steep manufacturing learning curve established in the last 20 years, the industry is experiencing continued cost/price

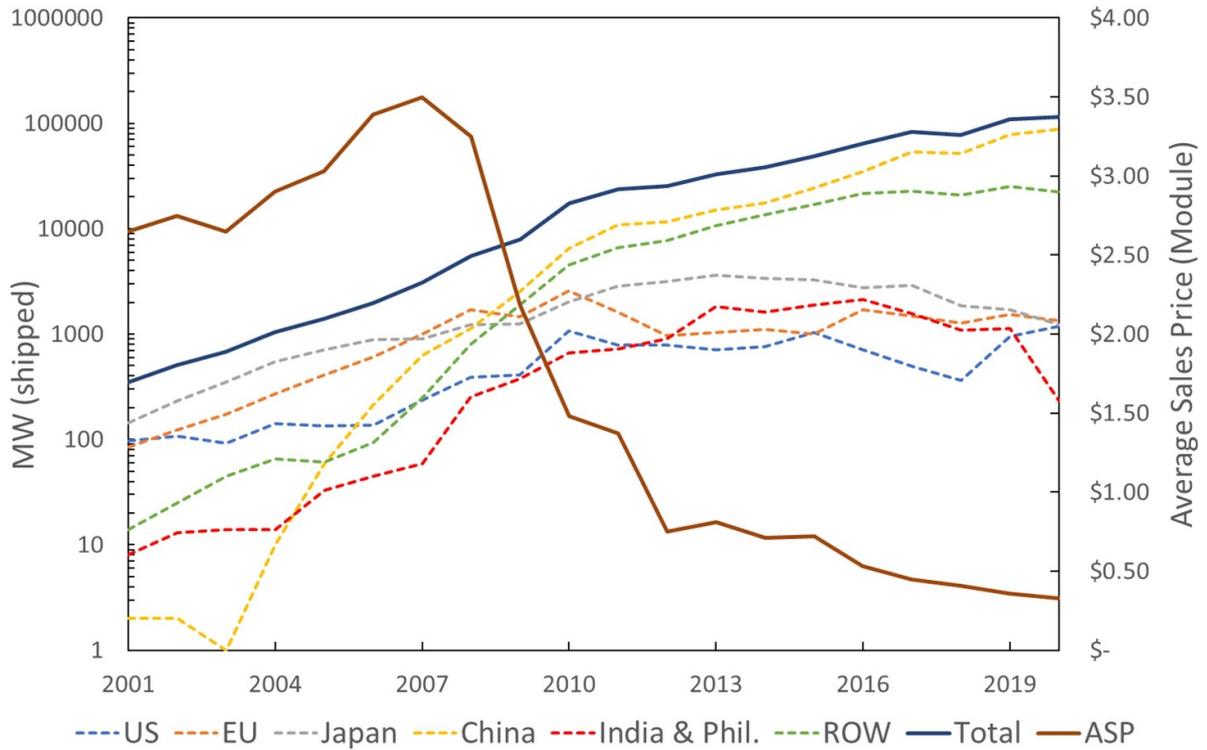


Figure 22. Country shipments of PV from 2001 to 2002 and average module sales price (ASP) at the first point of sale. Data provided by SPV Market Research [162].

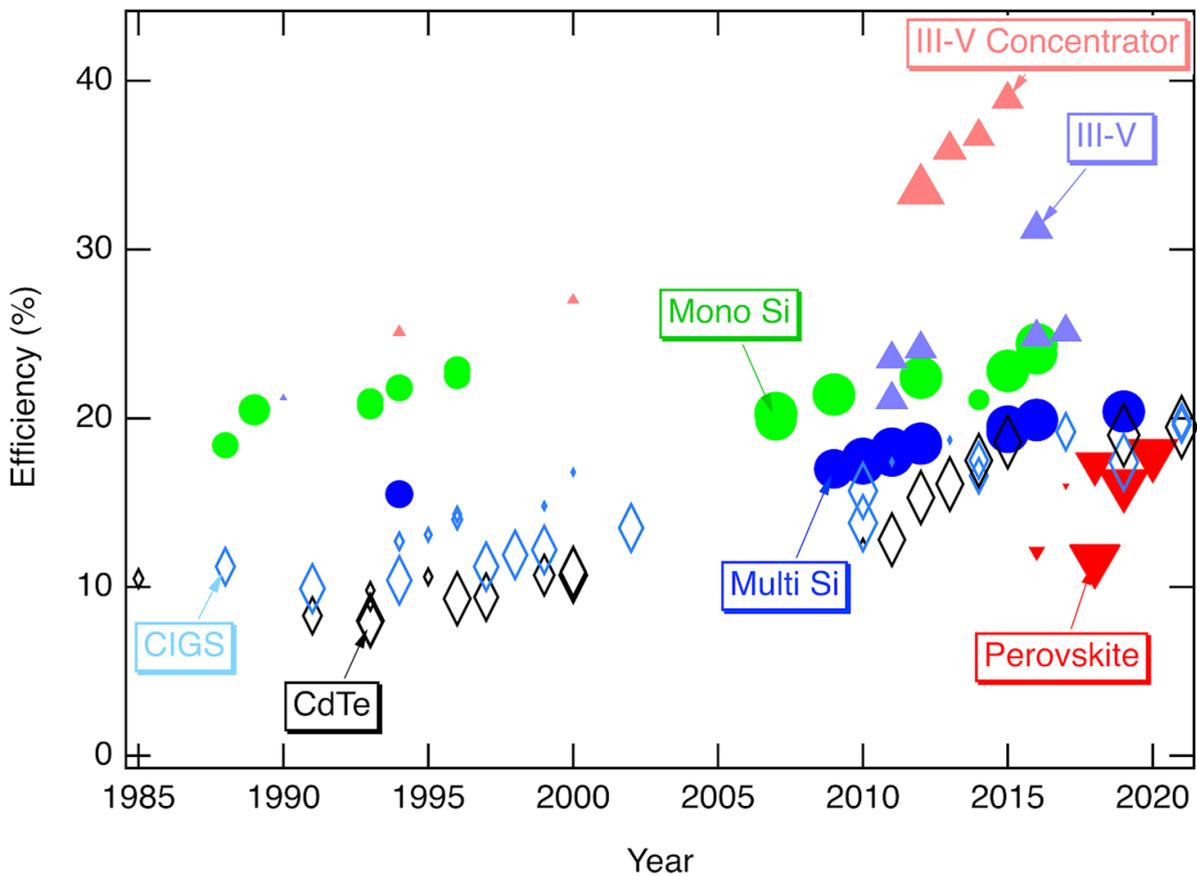


Figure 23. Champion module efficiencies as labelled with the size of the markers scaled by the log of the area with the smallest size marker being 16 cm² module and the largest 23 000 cm². Data taken from www.nrel.gov/pv/module-efficiency.html.



Figure 24. Monique Alfris, co-founder of Pollinate Energy, delivering lighting where it is most needed by bringing technology, finance and social enterprise to emerging markets. Image provided by Monique Alfris (Credit: Pollinate Energy).

decreases leading to continuously lower cost of electricity production from PV.

Ongoing technology development has ensured that PV will continue to be the cheapest sustainable electricity source in the low carbon future. Even with this success, there remain technical and socio-economic challenges to improve efficiency and lower costs, increase the lifetime of PV modules, reduce materials usage, improve sustainability, increase the uptake and adoption of PV for new applications, and maintain societal support. In these areas, women scientists, entrepreneurs and educators continue to play important roles.

Advances in science and technology to meet challenges

A number of teams across the world are focused on the next breakthrough c-Si cell technologies, such as top/rear contact (TopCON), silicon heterojunction (SHJ) and interdigitated back contact (IBC). All of these technologies, alone or in combination, have been demonstrated in the laboratory to have some of the highest efficiencies possible for single-junction c-Si devices, 26.0% for p-type TopCON [164] and 26.6% for a combined SHJ-IBC [165]. Delfina Munoz (CEA) led a team demonstrating large area devices with front and rear contacts with efficiencies better than 25% with a roadmap for cost-effective manufacturing in Europe. The promise of higher efficiencies with these technologies, along with lower CO₂

emissions manufacturing and production closer to use, have motivated a number of companies and entrepreneurs in Europe and the US to introduce new manufacturing initiatives. Walburga Hemetsberger (SolarPower Europe), is acting to support EU manufacturing of PV wafers, cells and modules. In the US, Kate Fischer (Sunflex Solar) is working to bring laser-welded IBC modules to market.

Reduction in raw materials usage, particularly of certain metals and other rare elements (i.e. Ag, In, and Bi), is key to the on-going sustainability of PV as a large-scale energy source. The key innovations here are in the development of busbar-less cells and new module interconnection technologies. Alison Lennon (UNSW) has been involved in reducing Ag usage in module interconnections and replacing it with plated Cu. Xiaojing Hao (UNSW) holds the efficiency record (11%) for CZTS, a form of thin film that uses only earth-abundant materials.

Mariska de Wild-Scholten (SmartGreenScans) has been performing PV life-cycle analysis for many years and her models continue to be used to motivate improvement of the circularity of PV. A key sustainability and economic issue is improving the lifetime of cells and modules. Ulrike Jahn (VDE Renewables, and winner of the 2021 Becquerel Prize) has been leading an international collaboration in the IEA PV Power Systems Task 13 for Performance, Operation, and Reliability of Photovoltaic Systems. Work on degradation due to impurities in silicon by Alison Ciesla (UNSW), Catherine Chan (UNSW), Mariana Bertoni (Arizona State University), and

Bianca Lim (ISF Hamelin) has led to improved reliability of modules and cells in the field.

Beyond single-junction devices, the recently emerged perovskite cell technology has the performance credentials necessary for realising high-efficiency multi-junction cells such as perovskite-Si tandems. Researchers working in this area include Kylie Catchpole (ANU), reporting record energy conversion efficiencies, and Anita Ho-Baille (University of Sydney), reporting record device durability and fundamental degradation mechanisms of perovskites. Olga Malinkiewicz (Saulle Technologies) has introduced an ink-jet printed flexible perovskite device for new applications, while Laura Hertz (Oxford) focuses on the photo-physics and carrier dynamics. Regarding other photovoltaic technologies, Adele Tamboli (NREL), winner of the 2018 IEEE PVSC Wenham Young Researcher prize, is working on III-V/c-Si tandem devices. Karin Hinzer (University Ottawa) has contributed significantly to the fields of nanotechnology and quantum dot solar cells.

Generating electricity as close as possible to the point of use will improve overall system efficiency and cost. The distributed nature of PV also brings new opportunities unique to this sustainable electricity source. It is a product that can be realized by large electricity companies, cities and municipalities, large and small businesses, homeowners, and individuals alike. Researchers and entrepreneurs all over the world are capitalizing on the low cost, small unit size and scalability in order to integrate PV into all kinds of objects like

buildings, infrastructure, consumer products, and vehicles. Bonna Newman (TNO) is helping to realize the integration of PV into the urban environment, particularly on-board electric vehicles. Angèle Reinders (University of Twente) leads design-driven research matching technology with applications. Women such as Monique Alfris (NABERS), co-founder of Pollinate Energy, focused on ensuring solar solutions for impoverished populations in India.

Concluding remarks

PV is an international story of innovation and technology development, dramatic price reductions and growing demand that is still playing out. Motivated by the opportunity to make a difference, women have played key roles in this science and technology development of PV.

In the last 20 years we have seen rapid and significant changes in PV technology. The next 20 years will bring even greater change as we transition to a zero-emissions future.

Solar PV currently provides 3% of the world's electricity but is projected to deliver close to 70% of by 2050 [166]. This growth will see even faster innovation, as economies of scale continue to drive solar to extraordinarily low costs and broader applications. Women can be expected to have an increasingly important role in the science and engineering of PV, as the technology delivers the lowest-cost, clean and renewable source of electricity.

14. Neuromorphic computing and devices

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Status

The research field of neuromorphic engineering dates back to the late 1980s to early 1990s, and the original definition was coined at Caltech (USA) by Carver Mead, referring to academic research dedicated to the understanding of how the biological neural networks work and trying to emulate them using transistors operated in their 'weak inversion' or 'subthreshold' regime. Misha Mahowald, as a PhD student at Caltech, first proposed the development of silicon retinas [167], stereo correspondence chips, and silicon neurons. Recently, the *Misha Mahowald Prize for Neuromorphic Engineering* was created to recognize outstanding achievements in the field and was first awarded in 2016.

Since the 2000s, the community has been growing and has started to use the term neuromorphic to describe mixed-signal and pure digital systems that could be used to simulate models of spiking neural networks (SNN) and/or to implement them in hardware, shifting towards application-driven research and proposing various large-scale neuromorphic computing systems. This effort was possible thanks to advancements in the CMOS-VLSI technology. Eustace Painkras was one of the key researchers who developed the SpiNNaker1 chip [168], which forms the basis of the million-core SpiNNaker machine located at the University of Manchester (UK). The Institute for Neuroinformatics in Zurich (INI, Switzerland) has been one of the world's major centres for neuromorphic engineering, working on novel circuit development for SNN. Shih-Chii Liu (University of Zurich) contributed to the development of real-time sensory systems [169], and Elisabetta Chicca (at INI as a PhD student, now at the University of Groningen, Netherlands) has been working since the early 2000s in the field of mixed-signal CMOS-based neuromorphic learning and sensory processing circuits [170]. Sylvie Renaud (Bordeaux University and IMS-CNRS, France) contributed to the development of artificial and biological hybrid network *in vitro* [171], analogue and mixed neuromorphic very large scale integration (VLSI), and hardware platforms of real-time SNNs.

Since 2008, the neuromorphic community has been joined by material and device physics by studying the properties of nanoscale memristive devices and trying to exploit their physics to implement neural and synaptic functions. Teresa Serrano-Gotarredona (IMSE-CNM, Spain) was one of the pioneers in proposing memristive devices as artificial synapses in neural networks [172]. The group of Barbara De Salvo (CEA-LETI, France) was among the first to develop memristive devices and experimentally demonstrate their potential as

artificial synapses [173]. The group of Ming Liu (Chinese Academy of Sciences, China) has been working to exploit the developed know-how in memristive devices for applications in hardware neural networks [174].

Current and future challenges

The current research field of neuromorphic computing has received a significant boost by exploiting the large class of memristive devices as new hardware building blocks able to reproduce neural behaviours, and then substituting or complementing CMOS circuits. Memristors can enable 'in-memory computing' in neural networks, thus overcoming the von Neumann bottleneck. In-memory computing will avoid energy costs associated with data transfer between memory and the processor, and finally render neuromorphic systems more brain-like. However, there are no large-scale architectures exploiting memristor technology and many recent advancements in neuroscience are still to be brought into hardware. Therefore, the main current and future challenge is the development of large-scale hardware systems that can exploit the physics of novel nanodevices and the advancements in theory and algorithms towards efficient, flexible and low power computation. To fulfil this goal, strong interdisciplinary research from material science and novel concepts are necessary, through microchip design and manufacturing, computational neuroscience and machine learning. Many women researchers are currently contributing and leading important efforts, but for the sake of space we only focus here on a few, non-exhaustive examples, mainly in the field of material sciences and nanodevices.

Regarding the advancements of material science with future impacts in the field of memristive devices and neuromorphic systems, we can mention the groups of Jennifer Rupp (MIT, USA), Beatriz Noheda (University of Groningen, Netherlands), Judith Driscoll (University of Cambridge, UK), and Regina Dittmann (FZ Juelich, Germany), working in the field of oxide-based memristive systems. Zdenka Kuncic (University of Sydney, Australia) is exploring neuromorphic dynamics in nanowire networks. Shifting from materials to devices, Julie Grollier (CNRS and Thales, France) is leading efforts in spintronic devices for bio-inspired computing [175], Ru Huang (Peking University, China) is investigating neural networks by integrating different memristive devices [176], and Sabina Spiga (CNR-IMM, Italy) is investigating oxide-based memristors as electronic synapses for SNN [177]. Elisa Vianello is now responsible for the embedded AI program at CEA-Leti, Grenoble, and she has contributed to the design and fabrication of neuromorphic circuits co-integrating advanced CMOS and memristors to implement synapses in artificial neural networks [178].

Advances in science and technology to meet challenges

To meet today's challenges of neuromorphic computing, it is necessary to join together many competences in neuroscience,

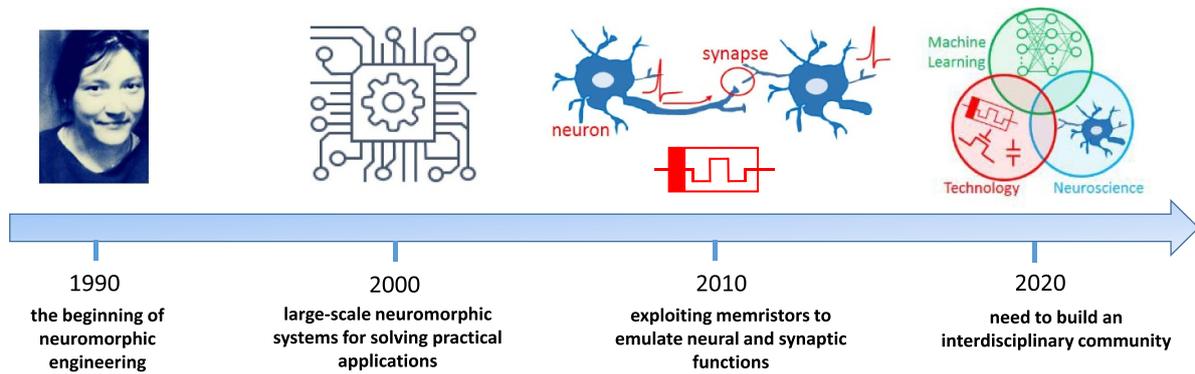


Figure 25. Schematic evolution of the main advancements and challenges in the field of neuromorphic computing as a function of time. The main novelty in term of technology research direction is highlighted for each decade (the indicated dates represent only a time frame). After 30 years of research, the field of neuromorphic computing is facing today the big challenge of developing the next generation of computing with a holistic approach, joining together neuroscience, machine learning and advanced technology. Many women have led and will continue to lead this research field, some of them cited in this work and many others not mentioned only for a lack of space. Photo of Misha Mahowald on the left. Credit: T Delbruck, Pasadena, ca. 1991.

AI algorithms, architectures, and material/device engineering. This holistic approach will trigger the implementation of new principles and new functions in power-efficient large neuromorphic systems, demonstrating at the same time their value in real applications. One of the key challenges is to develop neuromorphic systems that can interact with the real world, efficiently sensing and processing real-world sensory signals and natural multi-timescale data in real-time, e.g. for low-power and always-on internet of things (IoT) and edge computing.

Many women researchers are entering this field and are addressing novel materials or memristive device concepts, but there is also increasing interest in how to exploit memristive devices in real circuits/applications and/or how novel theory can be integrated in hardware towards new applications. In addition to the groups cited in the above sections, Silvia Battistoni (CNR-IMEM, Italy) is exploring organic memristors to mimic neuromorphic functions [179], Alice Mizrahi (CNRS and Thales, France) is working in the field of spintronic devices, and Yudi Zhao (Peking University, China) is working on the modelling-based co-design of memristors and neuromorphic circuits [180]. Duygu Kuzum (University of California, USA) is leading a group on nanoelectronic devices for neuro-inspired computing, and towards the development of neural interfaces. Regarding theory and algorithms, Eleni Vasilaki (University of Sheffield, UK) is leading a group developing computational models aiming to advance our understanding of brain learning mechanisms. Catherine D Schuman (Oak Ridge National Laboratory, USA) is working on evolutionary algorithms to train SNN. In terms of novel circuits and applications, Melika Payvand, Elisa Donati, and Charlotte

Frenkel (INI, Zurich) are working on the design of a new generation of ultra-low power, scalable spiking neuromorphic processors, based on mixed-signal processing and the integration of memristive devices [181]. The target applications are biosignal processing, smart sensors, and neuromorphic robots. Finally, Yulia Sandamirskaya (Intel, Germany) and Chiara Bartolozzi (IIT, Italy) are exploiting the neuromorphic engineering approach to enable the design of autonomous machines.

Concluding remarks

The field of neuromorphic computing already benefits from more than 30 years of research, with a significant increase in worldwide interest and the involved community in the last 10 years (figure 25). Research has broadened its focus from a pure academic environment to also include the industrial one, driven by many possible applications also directed towards future societal challenges (two major application domains are related to: (a) autonomous navigation and moving vehicles such as robots, drones and even cars; (b) sensor-based health-care and lifestyle systems). All new emerging memristive technologies and the tremendous advancement in the field of neuroscience, as well as machine learning, currently really need to be further developed with a holistic approach. Women have played an important role since the beginning and are continuing this role, also with the involvement of many young researchers in the field of novel material and device concepts, as well as their exploitation of energy-efficient neuromorphic computing systems for various applications, including bringing together the advancements provided by theory.

15. Nanophotonics and nanophononics

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Status

The nanophotonics and nanophononics fields aim at engineering and manipulating photons (i.e. light) and phonons (i.e. sound and heat) at the nanoscale, with great potential for advancing both fundamental understanding and new technologies. These fields have been greatly developed by the current astonishing capabilities of nanofabrication techniques, and they find an interface where light meets heat (see figure 26), leading to an interaction that certainly results in an interesting cross-fertilization with surprising effects.

The nanophotonics field aims at engineering/mastering of light–matter interactions by nanostructuring the propagating/interfacing medium. The field was most probably born from the desire of beating the diffraction limit in optical imaging. One breakthrough revolutionized how we envision interaction with light and nanostructures: the realization by Ebbesen and co-authors that sub-wavelength hole arrays could exhibit ultra-high optical transmission, not to neglect the discovery of photonic crystals. Ebbesen's finding went against physical intuition and opened the avenue to engineer matter at the nanoscale to manipulate the course of light. By carefully designing nanostructures, light can be focused, concentrated, diffracted and reflected in a dramatically unexpected manner compared to what one would expect with the effective medium theory [182]. The physical principles of nanophotonics have now been settled, revolutionizing the research areas of energy harvesting, quantum interactions and technology, optical communications, sensing, optoelectronics and optics. Prospects and challenges arise in the applied arena to deliver real applications and also thanks to the appearance of new materials such as the 2D van der Waals family.

The nanophononics field focuses on the investigation and control of phonons at the nanoscale, which are the dominant heat carriers in semiconductors and dielectric materials [183]. In many technologies, heat management has become the bottleneck for the development of next-generation devices. Interestingly, many works have shown the breakdown of macroscopic predictions of heat transport at the nanoscale, where extremely different phenomena can occur. This breakdown happens when critical dimensions, such as the size of the system and heat sources, or the distance over which heat is transferred, are comparable to the material's phonon mean free path [184]. Understanding phonon physics in such nanoscale systems is crucial for a basic description of energy flow in nano-systems, and for pushing technological applications such as

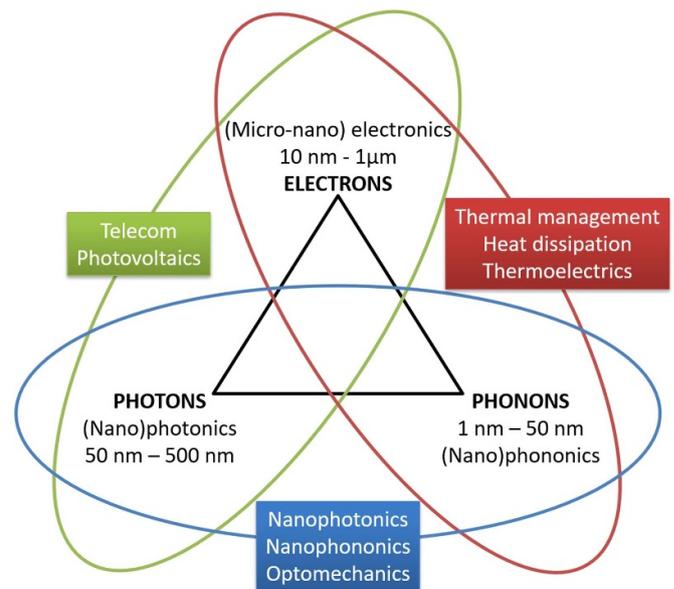


Figure 26. Overview of the nanophotonics and nanophononics fields. Photons and phonons meet each other at the nanoscale regime, giving rise to the optomechanics field. [185] Courtesy of J Ahopelto (VTT).

heat management in integrated circuits and optoelectronics, energy harvesting or PV. In this context, controlling phonons to the same degree as photons and electrons becomes indispensable.

Current and future challenges

While the basic physical principles of photonics have been established, there are still compelling challenges and perspectives ahead. Most photonic structures rely on highly regular and passive patterns. Non-periodic patterns and active structures offer new possibilities to engineer light–matter interactions. Calculations here are challenging due to the lack of periodicity; we expect AI approaches will increasingly open new horizons. This new kind of structure provide a way for photonic interaction enhancements. Other challenges are related to the fabrication of designs that become increasingly complex and have decreasingly small features. Also, 2D van der Waals materials offer a new world of possibilities in material combinations and functionality, but also a whole new set of challenges in nanofabrication and reproducibility.

One should also not forget the long-term sustainability challenge of nanophotonics, both in the nanofabrication approaches and in the use of scarce materials. This justifies the investigation of materials that include earth-abundant elements such as replacing Al in plasmonics or alternative absorbers in PV.

Interestingly, nanophotonics and nanophononics converge in two respects: in the interaction between light and mechanical motion, which is at the core of optomechanics, and due to the fact that the nanophotonics of long wavelength radiation is at the verge of meeting nanophononics by engineering heat management [186], a field in which there are

also theoretical and experimental critical challenges. Phonons, as quantized vibrations of the atomic lattice, are fully described by their phononic band structure or dispersion relation, $\omega(q)$, which provides a deep understanding of the material thermal properties, harmonic lattice dynamics, and the propagation of coherent waves. This can be accessed by techniques such as molecular dynamics or density functional theory calculations. Moreover, due to their dual nature, phonons can also be described as particles, which allows one to apply the Boltzmann transport equation (BTE) formalism to predict heat transport behaviour, new materials and phonon devices. However, solving the BTE for all phonon modes is a magnificent task and many efforts are currently devoted to simplifying it. One of the most remarkable challenges for these computations is the fact that phonons are bosons and, therefore, calculations should deal with the whole population of phonons over a broad range of frequencies, which makes it challenging to design a thermal device [183].

From the experimental point of view, mapping the whole dispersion relation and performing phonon transport measurements are extremely challenging experiments. The former can be done by inelastic neutron scattering, only accessible at a large facility and not suitable for nanosized samples, while the latter are typically affected by thermal contact resistance, unavoidable losses or very complicated modelling.

Advances in science and technology to meet challenges

There have been many remarkable experiments addressing these and more challenges in the nanophotonics and nanophonics fields led by women. To cite a few on the nanophotonic experimental side, Naomi Halas (Rice University) has led nanoplasmonics and material sustainability [187]. Jelena Vuckovic (Stanford University) included single photon emitters in nanophotonics to revolutionize quantum communication and sensing [188]. Jennifer Dionne (Stanford University) has demonstrated how the nanophotonics principles can lead to a better world by applying them to PV, medicine and biosensing. Silicon photonics owes its technological impact thanks to the work of Michal Lipson (Columbia University) [189]. Rachel Oliver (University of Oxford) has innovated the inclusion of nitrides in nanophotonics applications. On the experimental nanophononic side, Margaret Murnane (JILA—University of Colorado Boulder) led the uncovering of a new nanoscale thermal transport regime in semiconductors and dielectric materials in which, counterintuitively, nanoscale heat sources cool faster when placed together than when further apart [190]. Clivia Sotomayor-Torres's group (ICREA,

ICN2 Catalan Institute of Nanoscience and Nanotechnology) recently showed the crossover from a ballistic to a diffusive regime using thermal probe microscopy in graphene layers, as well as how phononic crystals are promising materials to reduce thermal conductivity. Marisol Martín-González's group (Institute of Micro and Nanotechnology—CSIC) is pushing thermoelectric performance by engineering nanomaterials [191]. Additionally, Pamela Norris' group (University of Virginia) employs transient thermoreflectance techniques to explore thermal boundary conductance. Simultaneously, there have been outstanding theoretical works also pioneered by women in the nanophonics field. For example, Sanghamitra Neogi (University of Colorado Boulder) studied surface nanoscale engineering on silicon membranes by using molecular dynamics [192] and Xanthippi Zianni's group (National and Kapodistrian University of Athens) performs Monte Carlo simulations to explore thermal properties on nanomaterials for thermoelectric applications. Other groups led by women combine both theory and experiment, such as Amy Marconnet's group (Purdue University), which explores the effect of coherent and incoherent phonon scattering in nanostructures and Zhiting Tian's group (Cornell University) that targets multiscale energy transport for diverse applications. Finally, in the field of optomechanics, at the intersection of nanophonics and nanophotonics, pioneering work is done in Eva M Weig's group (Technische Universität München), with an emphasis on dissipation, nonlinear dynamics, coupling and coherent control.

Concluding remarks

In the past few years, the progress in nanofabrication has enabled the design and realization of nanostructures that allow the control of light and heat transport, enabling a number of exciting experiments and opening the door to new technological applications. The progress and challenges of the nanophotonics and nanophonics fields are manifold and impact science and technology in multiple ways.

Several women have already made substantial contributions to these fields and have served as role models, supporting and guiding many young women scientists starting in these fields. This will certainly lead to a more balanced situation and encourage young generations to go ahead with their scientific and/or technical vision and dreams.

Data availability statement

No new data were created or analysed in this study.

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1. Plasma materials processing

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3. Super-resolution microscopy

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4. Bioelectronics

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6. Nanomagnetism

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8. Quantum materials: phenomena and devices driven by symmetry breaking

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9. 2D materials: synthesis and physical phenomena

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11. Opportunities and challenges in development of multi-valent batteries

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12. Fuel cells

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14. Neuromorphic computing and devices

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15. Nanophotonics and nanophononics

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