China's mark on materials

China's researchers have established themselves as important players in many areas of materials science. We asked several experts to discuss the history, present state and future outlook for their fields in China, including any barriers to further success. Disciplines such as condensed-matter physics, materials under high pressure and thermoelectric materials all have a considerable footprint in this country, and China's scientists contribute significantly to global efforts. Substantial investment in research infrastructure — including a growing microscopy and computational community, and the opening of China's first spallation neutron source user facility in 2017 — facilitates these achievements. One of the ultimate aims of materials science is of course to birth new technologies that can benefit society; China has taken significant steps towards aiding the commercialization of its research, with graphene being an early success story. Underpinning all these efforts is the ambition and capabilities of China's researchers, and determined government plans for future prosperity.

Unearthing new physics

Condensed-matter physics is one of the most active research topics in China. **Qi-Kun Xue** considers the reasons underpinning its success.

Condensed-matter physics (CMP) constitutes a major component of physics research in China, with around half of all physics faculty members in Chinese universities engaged in CMP research. Over the past 20 years or so, funding for basic research in China has enjoyed a double-digit annual growth rate on average, with CMP attracting considerable investment. As a result, CMP in China has experienced considerable prosperity, becoming the most widely practised subfield of physics research and perhaps the most competitive of all basic research disciplines in China.

A pivotal year that secured the rapid development of CMP was 2005, which saw the launch of the National Plan for Medium–Long-Term Development of Science and Technology (2006–2020). Quantum physics and information technology were selected as target areas for priority funding, to boost the likelihood of scientific breakthroughs. The Chinese CMP community seized this opportunity: during the 10 years that followed, achievements in CMP research were often highlighted in annual reports from the National Natural Science Foundation of China (NSFC) and the Ministry of Science and Technology (MOST), two major funding agencies for basic research in China. Topological insulators, high-temperature superconductivity, spintronics and strongly correlated systems of electrons were the four priority CMP areas during this period, and Chinese physicists played leading roles globally in some of these. Here, I discuss the reasons for the success of China's CMP research and offer an outlook for future developments.

The rapid rise in the quality and impact of research into CMP — and many other scientific disciplines — in China can be traced to its workforce: the number of capable and skilled researchers has benefited substantially from a wide variety of government-level talent programmes, which aim to expand the activities of skilled China-based researchers, as well as to attract capable researchers from abroad. These talent-fostering programmes are unique to China's funding system and are not found elsewhere.

Take the NSFC as an example: in 1994 it initiated the special category of Fund for Distinguished Young Scholar (Jie-Qing in Chinese) for researchers under the age of 45, which has established itself as one of the most successful talent programmes with a cumulative total of 3,004 individuals funded so far, receiving approximately US$0.6 million over 5 years. Scholars have been selected annually from skilled researchers across all disciplines of natural science and engineering for the past 20 years. Up to 2015, 228 physicists had won this honour, including 70 from CMP. In 2012, this successful programme was further extended to include junior researchers under 40 years of age in a companion Excellent Young Scholar Fund (Junior Jie-Qing), worth approximately US$0.2 million over 3 years. A combined total of about 600 Jie-Qing and Junior Jie-Qing scholarships are awarded each year, and these programmes have become the best avenues for universities to recruit faculty members, and for research institutes to recruit scientists.

The central government has stepped up its efforts to attract overseas scientists and engineers by initiating the Thousand Talents Program, which has been targeting overseas senior-level scientists from well-known research institutions since 2008. This scheme was extended in 2011 to include junior researchers in the Young Thousand Talents Program. Unlike earlier recruitment efforts, these two global talent programmes are open to everybody irrespective of nationality, and have been particularly successful in attracting Chinese researchers back from overseas. Out of around 4,500 'young talents' awarded so far, about 300 work on CMP. At Tsinghua

University in particular, a total of 131 young talents have joined, including ten in physics with five of these working on CMP. Large-scale recruitment efforts are also carried out by many provincial governments, and even local municipalities, through regional talent programmes.

A second reason for recent successes in CMP is improved research platforms. Led by funding agencies, substantial emphasis over the past 20 years has been directed towards establishing accessible laboratories with balanced regional distribution. A major step towards such shared platforms is the system of State Key Laboratories established by MOST. The annual budget for each laboratory runs at about US$1.5 million, with up to US$10.1 million available for upgrading facilities and instruments every 5 years. There are currently ten such State Key Laboratories in physics, five of which are focused on CMP. There are also national laboratories for synchrotron radiation, the upcoming China spallation neutron source and strong magnetic fields, among others, operated by different sectors of the government. As a further example, researchers from the Chinese Academy of Sciences (CAS) developed the world's first vacuum ultraviolet laser-based angle-resolved photoemission system (ARPES) in 2006, which afforded substantial insight into high-temperature superconductivity in cuprates, iron-based superconductors and materials with topological properties[1].

Several years ago, NSFC also joined these efforts by establishing a special funding scheme for major research instrumentation, aimed at fostering exploratory research and the development of instruments with new capabilities. This approach recognizes the significance of advanced instrumentation to scientific research, and has stimulated the development of original ideas and concepts. The total funding from this scheme over the past 5 years is already approaching roughly US$530 million, and physics-related projects have fared well, accounting for more than half of the total. A large fraction of them are in CMP, including facilities for super-intense lasers, advanced high-pressure and low-temperature studies, and high-resolution spatial and temporal MeV electron diffraction and imaging. Such capabilities — some of which are currently being built and commissioned — offer substantial opportunities for China's CMP community and help to motivate its researchers.

There are two project funding schemes that are particularly important to CMP: MOST's National Plan for Major Research Project in Quantum Control, and the NFSC's Single Quantum State Major Research Programme. These schemes focus on fundamental problems for developing next-generation information processing and storage technologies, and on characterization, detection and manipulation of single quantum states and their interactions, respectively. The MOST programme has resulted in the funding of 73 large projects from 2006 to 2015, with average funding being around US$3.8 million for each (with a combined total close to US$300 million). This scheme is now being continued with increased scope and funding. The NFSC funding programme lasts for 8 years; it started in 2009 and has distributed US$30 million of funding to smaller teams or individual investigators, making it the largest-ever research programme from NSFC. Both of these schemes are additional to regular funding programmes at the two agencies. These two projects are a third important reason for the rapid rise and success of CMP, as more than two-thirds of the funded projects are in CMP.

There are two recent research achievements from the China community that particularly stand out. First, in 2014 a paper from Jilin University predicted[2] that sulfur hydride (H_3S) would superconduct at about 191–204 K under high pressure (200 GPa), relying on a numerical computation-based theory. High-temperature superconductivity in the sulfur hydride was experimentally realized in 2015 by a German group[3], establishing a record transition temperature of 203 K for superconductors. On the experimental side, in 2013, a group at Tsinghua University, in collaboration with researchers at Stanford University and CAS, observed[4] the quantization of the anomalous Hall effect in the magnetic topological insulator $(BiSb)_2Te_3$, more than 130 years after the anomalous Hall effect was discovered in 1880. This experiment has since been repeated by other groups around the world. The reason that these two achievements stand out — beyond their scientific merit — is that the researchers involved all benefited from the various talent programmes, research platforms and facilities, and project-funding programmes discussed here.

The spectacular rise of CMP in China can be seen in the increased presence of Chinese physicists at international meetings and the rising number of influential research findings. Despite an apparent slowing of the growth rate of gross domestic product, the government has vowed to continue to increase funding for basic research. In the years to come, we can expect China's CMP community to play an ever-increasing role on this global stage. ☐

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China's first pulsed neutron source

The China Spallation Neutron Source is expected to produce its first beam in 2017. **Hesheng Chen** and **Xun-Li Wang** provide an overview of this user facility and what it means for science in China and elsewhere.

Neutron scattering is a powerful tool for materials researchers and industries. Over the years, it has made substantial contributions to many areas of physics, chemistry, biology, materials science and materials engineering. For example, neutron scattering played a crucial role in elucidating the interplay between spin fluctuations and superconductivity in high-temperature superconductors[1]. In addition, because of their characteristic energy scales, cold neutrons are uniquely positioned to probe dynamic processes in soft matter[2], where applications range

Figure 1 | Aerial photo of the China Spallation Neutron Source taken in April 2016. The facility is intended to be open for users from 2018. Numbering indicates the following: (1) linear accelerator (the actual accelerator is underground); (2) rapid cycling synchrotron; (3) the first target building and experimental hall; (4) main substation; (5) future site of the second target station; (6) offices and laboratories; (7) service building.

from consumer products to photovoltaic materials and drug delivery. Neutron scattering also offers fundamental insight into mechanical deformation at the atomistic level[3] and is likewise invaluable for assessing the integrity of larger engineering structures, such as bridges[4] and wheel hubs of high-speed trains[5]. Given these wide-ranging applications and complementarity to X-ray diffraction, the last few decades have witnessed rapid advances in neutron scattering sources and instrumentation. Most of these developments occurred in North America, Europe and, recently, in Japan[6]. Now, the establishment of the China Spallation Neutron Source (CSNS; Fig. 1) means that China is poised to become a key player.

The decision to locate the CSNS in the southern city of Dongguan, close to the border with Hong Kong, was strategic. Historically, major user research facilities have been located in Beijing, which has a high concentration of renowned universities and many top research institutes of the Chinese Academy of Sciences (CAS). When CAS began to develop the plan for a neutron scattering facility in 2005, it instead looked to the southern part of China, which was booming economically but had few large-scale research centres. In partnership with the local government, the goal was to elevate scientific research and technology development in the most economically active region in China, matching scientific development that had previously centred on cities in the north and east of the country. In the long run, these measures will also help to promote economic restructuring in the region by creating value-added, high-tech products.

The Institute of High Energy Physics, CAS, is tasked to plan, construct and operate the facility in cooperation with the Institute of Physics, CAS. The total construction budget is US$345 million. Following a detailed planning phase, the final technical parameters for the CSNS were approved in 2008 and construction work started in May 2012. Construction is scheduled to take six and half years to complete. Installation of the accelerator system is well underway, with the first neutron beam expected in September 2017 and the first users in 2018. The facility will be available to the global research community based on scientific merit, via a peer-reviewed proposal system. The CSNS has received enthusiastic support and valuable advice from the international community regarding the design and construction of the facility. Continuing this international exchange is vital to ensure that the CSNS remains at the forefront of the application of neutron scattering.

Three instruments have been planned as part of the phase I construction project: a general purpose powder diffractometer, a small-angle scattering instrument and a neutron reflectometer. These instruments, which take full advantage of a broad neutron beam bandwidth, are designed to address the most pressing needs of a growing user community working on structure determination at atomic and nanoscales. The broad bandwidth also provides opportunities for innovative instrument design. For example, chopper spectrometers for inelastic scattering measurements can benefit from a multiplexing design, utilizing multiple incident beam energies to cover a wide dynamic range, effectively increasing the performance of the spectrometer. At a source level of 100 kW, the initial three instruments will be competitive with their international counterparts (for example, in terms of the precision in structure determination or time resolution in kinetic studies). Upgrading the CSNS to 500 kW in the future, including a second target station, will extend the scope for cutting-edge research in both diffraction and spectroscopy.

As the first pulsed neutron source in China, the CSNS will provide research opportunities that have hitherto been inaccessible to the scientific community in the country. In preparation for its first experiments, the CSNS has hosted meetings with potential users from China and overseas to brainstorm ideas for impactful experiments that will be attempted as soon as the instruments are commissioned. Magnetic materials, which are of interest from both fundamental and applications perspectives, were a major discussion topic. It is recognized that sample environments, such as a high-field magnet that operates over a wide temperature range, will be key to enabling the anticipated experiments. In addition, energy materials, such as Li–ion batteries, catalysts, hydrogen-storage and nuclear materials are predicted to be among the early experiments. Recognizing the opportunities for world-class research offered by the CSNS, the scientific community in the nearby regions are also expected to be involved. The Dongguan Institute of Technology plans to create a centre for mechanical studies with neutron scattering as a primary tool, and South University of Science and Technology of China is developing plans for a high-pressure diffractometer at the CSNS.

Another major beneficiary of the CSNS is the scientific community of Hong Kong, where there have been steady efforts to promote the use of neutron scattering since 2013. For example, with support from the Croucher Foundation in Hong Kong, a biennial summer school was launched at the City University of Hong Kong to train highly promising postgraduate students and early-career scientists on the use of neutron scattering. In 2015, the first Gordon Research Conference on neutron scattering was held in Hong Kong, focusing on disorder in materials. In addition, a joint lab was founded by CAS and the Croucher Foundation to collaborate on neutron scattering science and technology. Discussions are also underway to build a beamline that is partially funded by Hong Kong at the CSNS. With these developments, Hong Kong is becoming a prominent centre for neutron scattering activities and a gateway to the CSNS.

Still, challenges remain. At present, only three instruments are under construction at the CSNS, although the facility can accommodate up to 20 experimental stations. More instruments are needed to increase the productivity to a level commensurate with the initial financial investment. A comprehensive instrument portfolio is also essential to provide the necessary tools to tackle diverse scientific and technology issues. Fortunately, planning is underway for additional instruments optimized for particular applications. Examples include an engineering diffractometer for residual stress studies, a chopper spectrometer for the condensed-matter physics community, a high-pressure diffractometer and a quasielastic scattering instrument for soft matter and life sciences. Multiple funding sources are being sought: from the central government of China, Guangdong Province, and the municipal governments in Dongguan, Shenzhen and Hong Kong. Immediate funding is also being pursued for a suite of state-of-the-art sample environments to support initial experiments.

The scientific infrastructure established by the CSNS will go a long way in promoting materials discovery and technology development in China. Already, it has attracted scientists to join universities and research institutions in the region and, over time, it is destined to become an international hub for materials research. ❐

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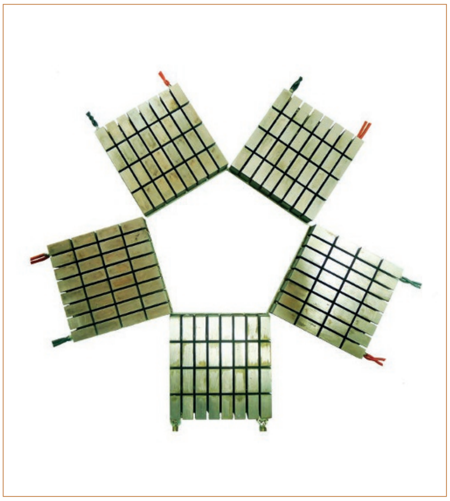
Thermoelectric materials step up

Xun Shi and **Lidong Chen** summarize recent progress in the field of thermoelectric materials in China, and discuss steps towards the realization of commercially viable devices.

Thermoelectric materials have the ability to directly convert heat into electricity and vice versa; electricity can be generated by applying a thermal gradient, while an applied voltage results in a cooling effect. Thermoelectric devices have the advantages of no moving parts, quiet operation, minimal environmental impact and exceptional service reliability. As a result of the global energy crisis and environmental impact of fossil fuels, these devices have attracted worldwide attention, and are likely to be of substantial benefit for specific applications (such as recovery of waste heat), rather than for primary energy generation[1]. Coupled with the rapid development of China's economy and major investments in scientific research, the study of thermoelectricity in China has grown substantially in the past two decades. For example, the number of thermoelectric-based projects awarded by the National Natural Science Foundation of China increased from 3 in 2000, to 59 in 2014, with a 50-fold increase in funding (data taken from www.nsfc.gov.cn). Nowadays in China, research activities in the field of thermoelectrics cover a wide spectrum, from basic research to device technology and industrialization.

A number of research centres in China have established expertise in the computational and experimental study of thermoelectric materials. For example, advances in the understanding of transport phenomena and the development of efficient simulation algorithms have enabled China's researchers to experimentally explore high-performance materials[2]. Examples of this can be seen in research efforts to understand and optimize the well-known 'phonon-glass' character of caged compounds, such as skutterudites and clathrates[3]. These caged compounds show a substantially lower lattice thermal conductivity and excellent thermoelectric performance by filling guest atoms into the intrinsic voids in the crystal lattice, thereby disrupting phonon propagation, and have been investigated for a number of years by researchers at the Shanghai Institute of Ceramics, Chinese Academy of Sciences (SICCAS) and Wuhan University of Technology (WUT)[4–6]. The filler's filling limit in caged skutterudites has been well explained and predicted by first-principles calculations, and thus provides a powerful guide to screen for new filled skutterudites[4]. Phonon calculations have also determined the vibrational frequencies of these guest atoms and, in turn, have been used to design double- and multiple-filled caged compounds with fillers with widely different vibrational frequencies, further reducing lattice thermal conductivity.[5] Thus, deep insight into their general physics has been gained by China's researchers via computational approaches. Given the growing investment in China into computational approaches for materials design, such methods for thermoelectric materials are likely to become even more prevalent. Moreover, the study of thermoelectric materials is one area of focus for the recently formed Shanghai Materials Genome Institute, which is sponsored by the Shanghai municipal government[7].

Looking beyond traditional options, China's researchers have also contributed to the discovery of new families of thermoelectric materials. For example, the 'phonon-liquid electron-crystal' idea can explain low lattice thermal conductivity in many Cu- and Ag-based



SHANGHAI INSTITUTE OF CERAMICS, CHINESE ACADEMY OF SCIENCES

Figure 1 | Skutterudite-based thermoelectric modules manufactured by the Shanghai Institute of Ceramics, Chinese Academy of Sciences. Each module has dimensions of 50 mm × 50 mm, and a maximum output of 25 W for a 500 K temperature gradient.

ionic semiconductors[8]. Attributed to the presence of liquid-like ions in these ionic thermoelectric materials, some of the transverse vibrational modes were shown to be eliminated, and extremely strong phonon scattering was observed[8]. Consequently, several new Cu- and Ag-based compounds with high thermoelectric performance have been reported, such as $Cu_{2-\delta}Se$, $Cu_{2-\delta}S$, $Cu_{2-\delta}Te$ and Cu_5FeS_4. Researchers at Beihang University and Tsinghua University have also been involved in national and international collaborations to demonstrate that large anharmonicity induced by crystal structures can lead to intrinsically very low lattice thermal conductivity, and thus good thermoelectric performance[9,10]. This has been successfully applied in the development of excellent thermoelectric materials, such as SnSe (ref. 9) and BiCuSeO (ref. 10). The study of organic materials for thermoelectrics is also becoming a highly active field in China, and thermoelectric properties have been demonstrated in a series of metal coordination polymers on account of their intrinsically low lattice thermal conductivity[11].

Thus far, this discussion has focused on the intrinsic physical factors that determine thermoelectric performance. It is also well-known that thermoelectric properties can be substantially improved by tailoring their microstructures — specifically, reducing grain size and introducing a nanoscale heterogeneous structure to tune electron and phonon transport — by appropriate synthesis and processing. Towards this goal, researchers at the University of Science and Technology of China and South University of Science and Technology of China have demonstrated that nanoscale homojunctions and heterogeneous structures can synergistically benefit electronic and thermal transport in $AgBi_{1-x}Sb_xSe_2$ (ref. 12) and BiAgSeS (ref. 13). Materials processing routes that can be scaled up are likewise necessary for commercial viability. These are important research directions in China, with active groups at WUT and Zhejiang University. By combining rapid solidification (melt spinning) with fast ingot consolidation (spark plasma sintering), nanostructured $Yb_{0.3}Co_4Sb_{12}$ possessing nanophases down to 10–20 nm embedded in the bulk matrix have been demonstrated, with an enhancement of thermoelectric performance[14]. Moreover, ultrafast, self-propagating high-temperature synthesis has been successfully applied to create a number of thermoelectric compounds[15], and a hot deformation method has achieved highly textured polycrystalline Bi_2Te_3-based materials with tunable nanosized grains[16]. An extreme case of microstructure control is $Cu_2S_{0.5}Te_{0.5}$, which has a mosaic grain structure and displays glass-like, ultralow thermal conductivity with charge carrier mobility equivalent to a crystal[17]. High-pressure techniques have also been used for material synthesis by a group at Yanshan University, having the advantage of generating metastable phases that are difficult to be realized by other synthesis approaches[18].

The continuous development of high-performance thermoelectric materials has enabled the design and fabrication of efficient thermoelectric devices for practical applications, and China is one of the global pioneers in this respect. As one of the best candidates for thermoelectric power generation, skutterudite-based modules have been manufactured and sold as commercial products at SICCAS (ref. 19; Fig. 1), with energy conversion efficiencies larger than 8% and service life longer than 10 years at working temperatures up to 500 °C under inert gas. Currently, SICCAS has the ability to produce approximately 1,000 skutterudite-based modules per year and is aiming to expand this to more than 10,000 per year in 2017. Due to constraints on budget and production capacity at SICCAS, module fabrication will be transferred to national or international companies for low-cost and large-scale production. Hybrid thermoelectric–photovoltaic power generators (up to 5 kW) and waste-heat recovery generators (up to 940 W) for cars and trucks have also been demonstrated by researchers at WUT. Right now, there are more than 20 companies in China fabricating Bi_2Te_3-based cooling modules and a few companies fabricating Bi_2Te_3-based power generation modules that work below 200 °C (at present, no companies have the technology for creating modules that operate above 300 °C). To further promote commercialization, China's government has set up national projects to fund facilitation of thermoelectric technologies for industrial applications, particularly for the recovery of automobile and steel plant exhaust heat, while external investment is also being sought.

The preceding discussion demonstrates that China is actively pursuing research projects that span the full development chain for thermoelectrics, from basic research to industrialization. And given the continued government investment into research of the relevant technologies, and successful attempts to demonstrate commercially viable working devices, China is likely to play a significant role in enabling thermoelectrics to meet their potential as a viable source of energy. ❐

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Boosting computational capabilities

Computational materials science has grown in China in recent times. **Hai-Qing Lin** gives an overview of China's efforts towards a Materials Genome Initiative and the challenges faced.

Due to the rapid development of computational physics and quantum chemistry as research disciplines since 1990, and enabling advances in computer technology and software, computational-based materials research is growing in importance. One of the most challenging issues in materials science is to identify materials with potentially good properties, out of thousands of candidates. The traditional approach, based on trial-and-error experiments, is time-consuming, resource-intensive and often fails to discover those materials with optimum properties. In addition, understanding the mechanisms behind how atomic and microscopic structures control macroscopic properties would significantly enhance search efficiency, aiding the prediction of complex materials' properties for advanced applications. Computational approaches towards materials science can offer substantial advances in this regard, providing shortcuts to new materials, and understanding of material behaviour. Given the substantial research and technological efforts towards materials science in China, it is no surprise that computational materials is a rapidly growing field in China.

Theoretical studies of materials properties in China started as early as the 1960s[1]. These initial works gave new insight into structure–property relations in functional materials (such as non-linear optical effects in crystals[2,3]), prompting the development of new materials. However, most calculations were based on empirical or semi-empirical approximate methods, which relied on experimental data. Likewise, computers were predominantly used to calculate and interpret properties of simple materials using approximations and to provide basic theoretical support to experimental studies. Since 1990, China paid greater attention to computational materials science: in 1992, the National Natural Science Foundation of China established a project for basic research into computational approaches for materials, significantly boosting the development of the field in China. Likewise, the Ministry of Science and Technology (MOST) set up national-level projects in 1997 and 2000, focusing on materials design and property prediction. By the end of the 1990s, advances in first-principles theory and computational capabilities had provided a better understanding of the fundamental properties of functional materials, enabling more advanced studies. Recently, with the development of new calculation methods and greater computing power, researchers in China are able to apply quantum mechanics to design complex materials with prescribed properties, which can then be studied experimentally[4–7]. China has a large and growing number of computational scientists at top universities and Chinese Academy of Sciences institutes, including dedicated centres such as the Beijing Computational Science Research Center.

Realizing the catalysing role that computational approaches can play in materials development, the United States has established a number of programmes, resulting in the Materials Genome Initiative (MGI) in 2011: the US federal government invested US$250 million with the aim of integrating materials computation tools with efficient experimental methods and databases for the design of advanced materials at an accelerated rate and reduced cost. Other countries have similar projects, such as Japan's Element Strategy and India's Mapping the Materials Genome.

In 2012, the Chinese Academy of Engineering and the Chinese Academy of Sciences launched related projects (the names of which translate roughly as 'materials science and system engineering development strategy — Chinese version of the materials genome project' and 'development of material genomics and materials science innovation') and in 2016 an equivalent to the MGI was launched, Key Technology and Supporting Platform of Materials Gene Engineering, which has the same aims and scope as its US counterpart. It is coordinated by MOST and comprises 40 projects, each granted US$4.6–7.6 million over 5 years. Areas of focus include high-throughput methods (computation, synthesis and characterization) and the development of materials databases, covering biomedical, energy, rare earth and catalysis materials, and special alloys. Moreover, MOST also set computation as a major research topic to promote research and technology development. These two programmes, Key Technology and Supporting Platform of Materials Gene Engineering, and High Performance Computing, will run for approximately 10 years and are part of the Made in China 2025 programme.

To ensure the future success of this growing community in China it is important to develop new computational methods and enhance computing power to extend predictive capabilities and accuracy. For example, we need more accurate functionals to predict bandgaps of semiconductors and related material properties — which are of great importance for new technologies in China — especially for more correlated *d* and *f* band systems and for excited states. More importantly, to accelerate the growth of the computational materials community in China, the research environment should be further improved. In particular, by making funding reliably available for 3–5 years to develop state-of-the-art first-principle algorithms and corresponding software, by collaboration with experimental groups, through adequate training for young researchers, and by encouraging scientists to understand and solve a problem — not just for publications. A particular concern here is that the discipline relies on new codes but recognition for the development of these is usually not included in researcher assessment (as opposed to papers published). Intellectual property protection is also an issue in China and researchers often prefer not to share computer codes. An advantage that China does have is that students are very capable at mathematics and simulation techniques.

Next, although it is important to raise China's global status in science, government funding agencies should not just follow hot topics, but should also pay close attention to the fundamental research of materials that have high potential for technological and economic impact. Examples are advanced quantum materials, high-strength and high-temperature alloys, catalytic materials, materials for energy and rare-earth magnetic materials. In all of these fields, computational approaches are highly beneficial. In addition, immediate attention should be on the computational study of mesoscopic materials by developing multiscale simulation techniques, particularly in electronics, because, for example, conventional approaches break down for nanoscale devices, and first-principles-based approaches are computationally costly.

Considering the importance and difficulties faced in this research field, the government should invest more in the necessary resources required for success, including platforms for high-throughput computational searches, rapid experimental synthesis and characterization facilities, and databases of material structures and properties. These features are all part of the MGI in the United States, and presents researchers with opportunities to take computational research to the next level. Although infrastructure is gradually falling into place, more will need to be done to ensure that computational materials science in China can be successful in obtaining improved materials.

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High pressure presses ahead

Ho-kwang Mao discusses the history of high-pressure research in China, and recent developments to ensure further success.

Pressure is a fundamental thermodynamic variable that can dramatically alter the atomic and electronic structure of materials, resulting in concomitant changes to their properties. Generation of static pressure greater than 100 GPa in diamond anvil cells, and a growing number of associated in-laboratory and large facility-based probes worldwide, enables a broad pressure-induced phase space to be explored. These developments have permitted new physical understanding of a range of phenomena, not limited to what is going on in the Earth's core and celestial bodies, and pressure-induced changes in elastic, electronic, magnetic, structural and chemical properties of materials. However, vast unexplored territory remains, and high-pressure research has substantial potential for unearthing new behaviours of materials. It therefore represents an attractive opportunity for China to demonstrate its capabilities in an international scientific field.

China has traditionally been very active in high-pressure research. This has been driven in part by China lacking natural diamond resources, yet some industries in China, including hard-rock drilling and high-precision machining, rely on diamonds for superhard tools, synthesized by high-pressure routes. Moreover, knowledge of the dynamic compression of materials is relevant to Chinese defence science. As such, high-pressure research was relatively well protected throughout the tumultuous years of the Cultural Revolution (1966–1976), when other academic research fields essentially came to a halt. China has since grown to be the predominant manufacturer of the world's synthetic diamond abrasives.

To sustain the rapid economic growth experienced in China over the last few decades, international competitiveness in basic science has become increasingly crucial, and funding from the Chinese government towards this goal has been substantial. Materials science holds significant potential in this regard, and high-pressure research contributes to materials applications in three aspects. First, useful high-pressure phases, such as superhard diamonds and cubic boron nitride, can be synthesized directly under compression and preserved for ambient applications. Second, knowledge gained in high-pressure research may lead to alternative routes for the design and synthesis of high-pressure phases with useful properties. For instance, large single-crystal diamonds with ultrahigh purity can now be synthesized under low pressures using methods based on chemical vapour deposition[1]. Third, the ubiquitous impact of pressure on physical behaviour provides an indispensable shortcut for advancing basic understanding. Thus, high-pressure research has stood out as one of the key directions of study that the Chinese government is supporting.

CHAOHUI WU, XIAOLI XIAO AND YIBO ZHANG OF CHINA ARCHITECTURE DESIGN AND RESEARCH GROUP

Figure 1 | An artist's impression of the Center for High Pressure Science and Technology Advanced Research headquarters that is currently under construction in Beijing (due to be completed in October 2017).

Resultantly, Chinese research institutions and universities are making seminal contributions to high-pressure science and technology. For example, the National Key Laboratory of Shock Wave and Detonation Physics, China Academy of Engineering Physics studied the density and sound velocity of Fe–O–S alloys under extreme pressure–temperature conditions, leading to the suggestion that the Earth's liquid outer core is depleted of oxygen[2]. Meanwhile, researchers at the Institute of Physics, Chinese Academy of Sciences investigated the effect of pressure on the superconductivity of newly discovered doped iron chalcogenide superconductors[3,4], reporting a high re-emerging critical temperature of 48 K, the largest yet observed in this material class.

Jilin University has established itself as the leading high-pressure research centre in China since the 1960s. They recently made the astonishing discoveries that pressure could transform elemental sodium from a free-electron gas metal to a transparent insulator[5], and that pressure could crush C_{60} cages to form a new type of material with long-range ordering of short-range, disordered carbon clusters[6]. Meanwhile, researchers at Yanshan University made breakthroughs in the high-pressure synthesis of ultrahard nanotwinned cubic boron nitride[7] and nanotwinned diamond[8], and researchers at Zhejiang University reported pressure-induced devitrification of Ce_3Al — a seemingly disordered metallic glass — to a single crystal[9].

To build on and accelerate advances in China, the Center for High Pressure Science and Technology Advanced Research (HPSTAR) was established as a top team of the Chinese Thousand Talents Program in 2013. It is modelled after the Carnegie Institution of Washington, with the same mission statement of supporting exceptional individuals to encourage investigation, research and discovery in the broadest and most liberal manner (www.carnegiescience.edu/about/mission). HPSTAR is strategically set up with its central laboratory in Beijing (Fig. 1) next to the Beijing Computational Science Research Center, with the Shanghai laboratory next to the Shanghai Synchrotron Radiation Facility, and a further branch on the Jilin University campus. In addition, there is a virtual laboratory consisting of a team of scientific staff employed by HPSTAR, who collaborate with synchrotron facilities around the world to pioneer cutting-edge high-pressure X-ray technology. They devote significant time and equipment on-site, forming a large network in the United States and in Asia, providing HPSTAR scientists with ample access to major synchrotron facilities.

HPSTAR adopts common practices, which enabled some of the aforementioned breakthroughs, namely theoretical–experimental interaction, interdisciplinary approaches, international collaboration and utilization of central facilities crucial for high-pressure research. Including those mentioned previously, these practices have already resulted in a number of discoveries: observation of dislocation flow in 3-nm nickel crystals, in contrast to previous theoretical predictions that dislocations would be inactive for crystals below 10–30 nm[10]; measurement of the pressure-induced change of dihedral angles of molten iron in a crystalline silicate matrix via a 30-nm X-ray tomography probe, simulating the formation mechanism of the early Earth's core[11]; development of a new X-ray microprobe integrated with multigrain crystallography, used for the discovery of a key mineral at the Earth's core–mantle boundary[12]; and discovery of a new FeO_2 phase which may provide an explanation as to the origin of our oxygen atmosphere[13].

HPSTAR's open, flexible and liberal research system is alien to the rigid Chinese system, and has thus faced numerous hurdles, including visa and work permit obstacles for foreign staff, and residency requirements for Chinese employees on the municipal level. Nevertheless, it has thus far proven to be an effective system for significant breakthroughs, and has gained strong support from the Chinese central government, and more widely from the scientific community. Of particular note is that HPSTAR has been successful in attracting international researchers with non-Chinese origins, something that has traditionally been difficult to achieve in China, yet seen as important in diversifying the researcher pool in the country.

China has established itself as a strong figure in high-pressure research, providing a striking example of how China-based research groups can influence and lead global scientific research efforts. With substantial investment in many of the key facilities needed for high pressure research — including the China Spallation Neutron Source that is currently under construction — and an ongoing drive to attract the best researchers, China is in an excellent position to play a key role in advancing high-pressure science and technology, providing these enabling trends continue. ❐

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Microscopy sparks development

Electron microscopy has seen a massive boom in China. **Ze Zhang** and **Xiaodong Han** discuss what this could mean for materials research and development.

China's rapid development over the last few decades has led to the production of huge quantities of materials, for both domestic and international markets. For example, China accounts for more than half of the worldwide production of materials such as ferrous and non-ferrous metals, concrete and synthetic fibres[1,2]. However, due to a lack of exact microstructural control, or a complete understanding of the underpinning science, China has been unable to produce many high-end materials. Thus — at considerable cost — China must import millions of tons of high-quality specialty steels each year[3]

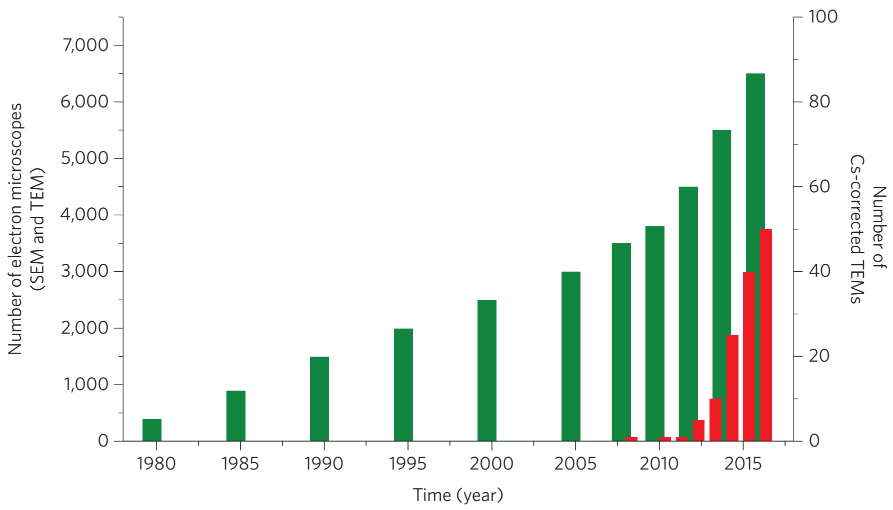

Figure 1 | Number of electron microscopes in China. The first electron microscope was introduced to China in 1959, with the first spherical aberration-corrected transmission electron microscope (Cs-corrected TEM) in 2008. SEM, scanning electron microscope. (Based on unpublished data from the Chinese Electron Microscopy Society).

as well as large quantities of high-purity semiconductor materials for electronics and alloys for transportation and aerospace. Furthermore, production processes requiring substantial energy input, and with low efficiency, have resulted in serious environmental problems including high levels of pollution in major cities and in the more industrialized provinces in northern China. These challenges call for some readjustment of the structure of industry in China, requiring that large gaps between manufacturing industries, research institutes and universities be bridged. To enable this, microstructural control is key, for which comprehensive facilities and expertise in electron microscopy are needed.

The development of advanced materials relies on smart design and precise engineering, necessitating that multiscale microstructural control be integrated with fundamental science. Determining correlations between materials' properties and their microstructures is crucial, and accurate structural characterization with atomic resolution — over multiple scales in spatial and chemical dimensions — is mandatory. Due to the rapid development of electron microscopy, high-resolution images with picometre precision, and chemical bonding information with meV energy resolution[4], can be approached. In fact, in countries with highly mature materials production technology, the precise characterization of material microstructures has long been a key enabling step in linking materials research with industrial manufacture.

The number of microscopes in China lagged behind the international microscopy community throughout the 1980s, but has developed rapidly since then (see Fig. 1). At present, there are more than 6,000 electron microscopes across 300 universities and research institutes in China, including approximately 2,000 transmission electron microscopes (TEMs) and more than 50 state-of-the-art spherical aberration-corrected high-resolution TEMs. In comparison, the United States and Europe each possess more than 200 and Japan about 100 aberration-corrected TEMs (based on unpublished estimates from the Chinese Electron Microscopy Society). The establishment of several electron microscopy research centres at Zhejiang University, Southeast University, Shanghai Jiaotong University, Chongqing University and Xi'an Jiaotong University during the past decade supplemented the well-established groups at the Beijing Laboratory of Electron Microscopy, Chinese Academy of Sciences (CAS) and the Institute of Metal Research, CAS, which became well-known internationally for the early discovery of quasicrystals by TEM[5]. The installation of a spherical aberration-corrected high resolution TEM at Tsinghua University in 2008 initiated sub-ångström-scale microscopy in China[6].

Of course, having a large number of high-end electron microscopes does not necessarily result in compelling research. Instead, well-trained operators and an interesting material or phenomena to study are vital. To help address these points, different national and local microscopy training schools and programmes have been working with microscopy companies, covering basic and advanced skills. In addition, numerous highly skilled and knowledgeable young microscopy scientists have returned to China in the past ten years from research institutes and universities abroad, via programmes such as the National Outstanding Young Scientist Foundation and Thousand Talents Program. Subsequent research highlights from the electron microscopy community in China include elucidating the mechanisms of twinning-enabled ultrahigh strength and ductility in Cu and Mg alloys[7,8] and a direct demonstration of the ferroelectric flux-closure domain structure[9], to name a couple. Additionally, *in situ* characterization of chemical, optical, electrical, mechanical and other physical properties is particularly active in China[10–13].

Realizing the importance of electron microscopy, research funders such as the National Natural Science Foundation of China (NSFC), the Ministry of Education, the Ministry of Science and Technology and CAS have invested intensively in recent years. For example, China's national 973 Program supported projects at leading microscopy groups during the past 10 years that aimed to develop novel microscopy techniques for cutting-edge research into areas including nano-, functional and structural materials. NSFC has likewise provided financial support for hundreds of projects[14,15] in universities and research institutes. Many of the aforementioned microscopy research centres collaborate nationally and internationally, as well as with industry. As such, the Chinese microscopy community has seen rapid growth and development in recent years, and boasts some of the worlds' leading facilities for materials characterization.

However, the lack of a China TEM manufacturer may slow down the development of new and advanced microscopy techniques that meet the specific needs of the Chinese research community. The in-house development of novel microscopy attachments and experimental cells may compensate for this. For example, an atomic-scale mechanical microscopy technique was developed at Beijing University of Technology[12,13] that allows for *in situ* atomic-scale dynamics of microstructure deformation to be captured. Previously, such information was only available by computer simulations and theoretical calculations. Likewise, NSFC and the Ministry of Science and Technology supported numerous projects to encourage the development of scientific instrumentation[14,15], including *in situ* systems for high-temperature multiscale mechanical testing[15] and ferroelectric, elastic and magnetic property correlation[14].

Finally, outstanding challenges remain that must be addressed to ensure that microscopy can play an increasing role in material development in China. For example, although allowance for microscopy is incorporated into funding for materials science, physics, chemistry, energy, information and environmental sciences, and others, more links between the microscopy community and scientists working in the aforementioned disciplines must be constructed. Likewise, a major concern is that the critical role of microscopy in materials development may not have been fully realized in industry and commercial research institutions, stunting new developments. Further efforts to fill these gaps are necessary, including attracting more microscopists to work on developing advanced materials. That being said, the facilities and expertise that have become available in China over the last few decades mean that microscopists will be increasingly able to contribute to the development of improved materials, which are relevant to the country's continued economic growth. ❐

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Graphene commercialization

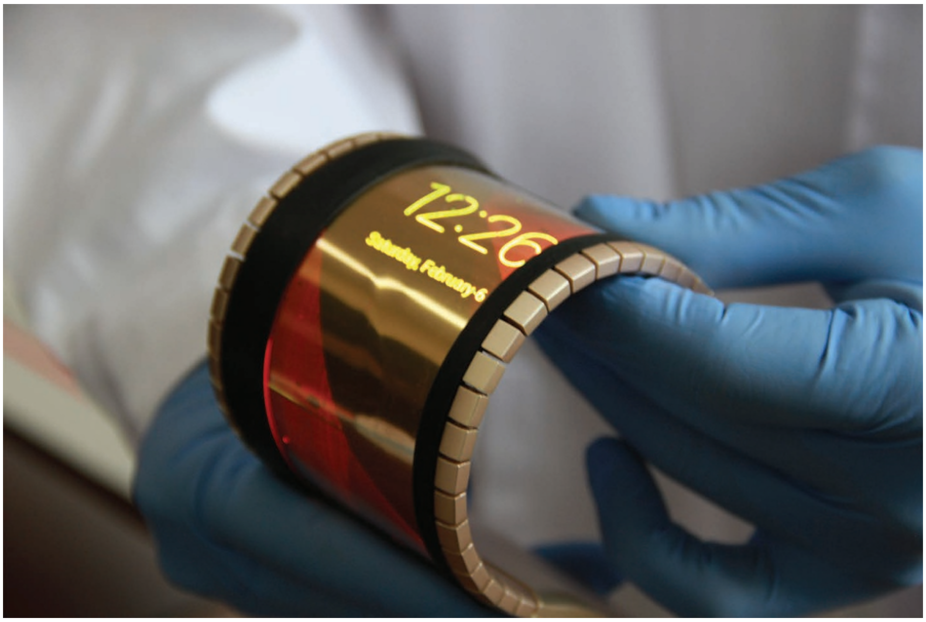
Graphene is extensively researched in China. **Xiaoyue Xiao**, **Yichun Li** and **Zhaoping Liu** illustrate how the China Innovation Alliance of the Graphene Industry aims to harness this for commercial opportunities.

Graphene receives substantial interest, driven by the unique physics it presents and a plethora of properties that make it attractive for applications. In particular, high in-plane conductivity, carrier mobility, transparency, flexibility and strength means that graphene has potential for implementation in a range of functional electronic devices, and for energy harvesting and storage, sensors, optoelectronics, composites and so on. Consequently, substantial efforts have been focused towards its research and development (R&D), with particular activity in the United States, Europe, South Korea and Japan. Likewise, the Chinese scientific community has invested considerably in this area. Until 2014, the National Natural Science Foundation of China (NSFC) awarded more than US$60 million to cultivate R&D projects on graphene and its related technologies (based on data collected by the China Innovation Alliance of the Graphene Industry). By the end of August 2015, China had published 34% of all papers on the topic, more than the United States (19%; ref. 1). But China also has big ambitions for the technological transfer of graphene from basic research to commercial products; local patents from China for graphene technology account for 38% of all graphene patents worldwide[2].

To stimulate technological transfer from laboratory to manufacture, the China Innovation Alliance of the Graphene Industry (CGIA) was established in 2013 by the China Industry–University–Research Institute Collaboration Association, which is owned by the Ministry of Science and Technology. Policy support is also supplied by them and a number of other government departments, with financial support from the major research funders in China. CGIA has constructed a platform to work with most of the major universities and companies that are engaged in graphene R&D, manufacture and investment, including Huawei Technologies Co. Ltd. (the world's largest manufacturer of telecommunications equipment). The broad aim of CGIA is to support the commercialization of graphene in China. This includes guiding policymakers who plan to work on graphene (for example, advising on which areas of graphene research local government should focus on, and the set-up of relevant infrastructure and companies), co-establishing geographical centres of excellence in graphene research and innovation, organizing international conferences, publishing patent reports and working on standardization protocols (such as the definition of graphene-related materials). Of course, securing investment funding for new companies is critical and the China Graphene Investment Alliance (part of CGIA) helps aid this. Also, CGIA cooperates with other countries, including Spain, Italy and Sweden.

A notable example of how CGIA has contributed to the graphene community in China can be seen in the support provided for local governments to create graphene industry parks. These are geographical centres that bring together the relevant people and infrastructure needed to determine policy, to develop the graphene industry in China and to attract investment. Importantly, supply chains for the manufacture of graphene from raw materials have been established at these parks as well as at downstream companies focusing on graphene applications, and at analytical service labs. Financial support from both local government and venture capitalists enables spin-off companies from universities and institutes to be based in the graphene industry parks, and facilitates their subsequent growth.

The largest of these is the Changzhou graphene industrial park established in 2013,



HAOFEI SHI, CHONGQING GRAPHENE TECH. CO., LTD.

Figure 1 | Flexible graphene-based smartphone produced by Chongqing Graphene Tech. Co., Ltd.

covering an area of 6 km^2. Located at this site is the Jiangnan Graphene Research Institute, which was set up with US\$300 million of funding and focuses on applied graphene research. Currently there are more than 70 companies in the park, forming a regional graphene industry cluster. Examples of these include Sixth Element, which produces graphene powder at a capacity of 100 tons per year (used for corrosion-resistant coatings, and in composites such as polyester resins and rubbers), and 2D Carbon, which manufactures graphene thin films (with a production capacity of 50,000 m^2 per year) for touch-panel and wearable electronic devices. CGIA's international cooperation centre is also located here with the aim of promoting bilateral cooperation committees with European and Asian countries. Likewise, two other graphene industry parks exist in Wuxi and Qingdao, supported by their respective local governments. The largest investment so far has been made by Shanghai Nanjiang Group, which separately gave US\$37 million in 2012 and 2013, and founded Ningbo Morsh and Chongqing Moxi with the help of the Chinese Academy of Sciences. Now, Ningbo Morsh is the leading graphene powder producer (used for Li–ion batteries and supercapacitors) with a capacity of 300 tons per year, and Chongqing Moxi is the leading graphene film producer (used for touch panel and wearable electronic devices; Fig. 1) with a capacity of 1,000,000 m^2 per year.

2015 was a landmark year for graphene commercialization in China: a Chinese producer of smartphones sold its first batch of two thousand smartphones that featured a graphene-based touch panel[3]; a new graphene-based lubricant as an additive in engine oil increased oil lifetime from 1,000 miles to 5,000 miles for sea-going freighters[4]; and a graphene-based capacitor was used for buses[5,6]. A number of companies are now producing graphene, in various forms, and in amounts of up to thousands of tons per year[7,8]. For electronics applications, Huawei Technologies Co. Ltd. aims to use graphene to prevent heat build-up on computer chips in smartphones and field base stations.

As China attempts to sustain its rapid economic growth, new challenges will be faced. Firstly, consensus suggests that it is important to reduce the cost of graphene-based materials: high material costs make establishing downstream products — and a commercial market — difficult, while the current low sales of graphene products means mass production is not justified, thereby keeping the price of graphene relatively high. Therefore, supporting downstream companies focusing on applications is essential. Secondly, graphene material standards (such as minimum property requirements and reliability of product quality) are not established, resulting in disorderly competition. Likewise, companies should be clearer about the performance of their products, and for which applications they might be used.

To ensure the continued development of a strong applications base for graphene, and to speed this process up, in November 2015 a document was co-published by several government departments, stating that now is a critical time for commercializing graphene[9]. It comments that by 2018 a chain of R&D and graphene manufacturing leading to commercial products should be built up, and that by 2020 graphene manufacturing should become well established in China with approximately ten competitive companies, and three to five world-leading innovation organizations, for example, world-leading R&D centres, and technology and engineering centres for graphene applications. A focus on applications that is not limited to energy storage devices, functional coatings, reinforced rubbers, sensors and flexible electronics is encouraged, and a forecasted revenue of up to US\$150 billion is predicted for graphene-related products by 2020. Lastly, the document emphasizes the importance of international cooperation for graphene applications, including global investment, joint ventures between Chinese and foreign capital companies, and global supply chains. CGIA is helping to achieve these goals, particularly regarding the graphene industrial parks and international cooperation.

Graphene commercialization is building considerable momentum in China. CGIA is well-placed to facilitate the transition of graphene from fundamental research to an important component in commercial products, and in future years will focus on helping the government to establish an ordered and competitive market for graphene. ❐

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