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EDITORIAL

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Moving mechanochemistry forward

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Arguably mechanochemistry is one of the oldest, and at the same time one of the newest, areas of chemistry. One of the oldest, because it has been theorized that early hominids were able to develop rapidly due to their ability to heat and mechanically process their food to make it easier to digest. Old, because the ancient Greeks knew that mechanically activating stones (consisting of cinnabar) with vinegar in a copper pestle and mortar caused them to convert into mercury.[1] We might be forgiven for thinking that this could have led our alchemical forbears to wonder if there were other stones that might also be persuaded to convert into gold. Early chemical luminaries such as Michael Faraday[2] and Wilhelm Röntgen[3] dabbled in mechanochemistry. However, in the late 19th and early 20th centuries, the field developed separately in many areas. Perhaps most significantly, synthetic chemists realized that reactions could be carried out with surprisingly high yields and selectivities by shaking them in a ball mill, and that they could even make novel compounds that their colleagues just using heat were not able to. Physicists were mechanically rearranging atoms into new configurations (*i.e.*, doing chemistry) using exotic means such as atomic force microscope tips and optical tweezers. Scientists and engineers studying the formation of lubricious and anti-wear films realized that they were mechanochemically formed. Biochemists found molecular motor proteins, such as myosin and kinesin, that were able to convert chemical energy into motion or, *vice versa*, mechanical energy into the biochemical energy storage molecule adenosine triphosphate. In 2023, this confluence of advances convinced the Royal Society of Chemistry that the time was ripe to establish a new journal dedicated to the field of mechanochemistry. It is rare that a journal has the privilege of helping to create a new sub-branch of chemistry but, having done so, it has the obligation of helping to define the field and, optimistically, suggesting how the field might develop. This editorial has two major goals. The first is to bring to the attention of the scientific community the challenges faced by the field to set people thinking about how they might contribute and, second, to form the basis for more thorough discussions in the future. The sub-topics below outline current thoughts brought forward from members of our editorial board. We lay out areas and topics here with the intent of establishing a new editorial series, which we invite the community to contribute to, and outline topics and hopefully lay out challenges, which will enable us as a community to come together to move mechanochemistry forward.

A. Fundamental mechanochemistry

A.1. Single-molecule activation

Mechanochemical transduction is a unique intersection of matter and energy, where the energy driving chemical change is sourced directly from mechanical work, defined as the dot product of force and displacement. This direct input breaks from the limitations of stochasticity typical of thermal and photochemical processes, allowing mechanochemistry to guide specific molecular transformations through directed atomic displacements.[4] In classical mechanics, two types of stress—normal and shear—provide distinct modes of action for selectively controlling displacement. Normal stresses, which act perpendicularly to an interaction plane, encompass both tensile forces (tension) and compressive forces (compression). Tensile forces align naturally with dissociative transformations,[5] while compressive forces promote associative processes,[6] both commonly exploited as normal stresses in mechanochemistry. Biological enzymes may have evolved to balance both normal and shear stresses to modulate

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reaction pathways,[7] demonstrating nature's ability to integrate these forces to accomplish complex transformations.

Shear stresses, defined as resulting in forces parallel to an interaction plane, introduce a complementary form of directional control that has been explored, but is not well understood and not especially well controlled.[8] Shear is typically associated with sliding surfaces and tribology, where it plays a critical role in processes such as friction, lubrication, and wear.[9] Intriguingly, shear is well-suited for concerted transformations, enabling simultaneous associative and dissociative changes, such as inducing bond breaking and formation in a single step. In synthetic polymers (see Section B.3), molecular-scale shear has been used in clever ways, such as with knots[10] and rotaxane dethreading,[11] but generalized approaches remain challenging. Moving beyond traditional methods, we envision a future where scalable, nanoscale devices could selectively manipulate atomic displacements. By applying both normal and shear stresses with high precision, these innovations have the potential to revolutionize chemical transformations with assembler-like precision across diverse molecular landscapes.

A.2. Experimental methods in mechanochemistry

Experimental methods in mechanochemistry have advanced significantly over the past decades, offering innovative approaches to harnessing mechanical energy for chemical transformations.[12] The ball mill remains a fundamental tool, providing controlled mechanical input through impact and shear forces.[13,14] Recent developments in *in situ* monitoring techniques have revolutionized our ability to observe mechanochemical reactions in real time.

Building on these advancements, synchrotron X-ray diffraction and Raman spectroscopy have emerged as powerful tools for elucidating reaction kinetics, and identifying intermediates and structural changes during milling. These techniques have revealed unexpected behavior in mechanochemical reactions, challenging initial assumptions about reaction mechanisms and kinetics.[15]

As our understanding of mechanochemical processes deepens, efforts to scale up these reactions for industrial applications have intensified. Continuous-flow mechanochemistry represents a significant advance in scalability and process control.[16,17] Twin-screw extrusion and resonant-acoustic mixing[18,19] are two examples of techniques that translate batch processes into continuous ones, potentially revolutionizing industrial applications of mechanochemistry.[20–22] The versatility of mechanochemistry has led to its integration with other fields, resulting in innovative hybrid methods. Mechanoelectrochemistry combines mechanical stirring with electrochemical processes, while mechanophotochemistry explores synergies between mechanical forces and light-induced reactions.[23]

As the field develops, standardization of experimental protocols and reporting practices has become essential. Efforts are underway within the mechanochemistry community to establish guidelines for carrying out reproducible mechanochemical experiments and addressing variables such as grinding frequency, ball-to-powder ratio and atmospheric conditions.

Mechanochemistry is transforming our understanding of chemical reactions and providing new, often more sustainable, approaches to material synthesis and chemical manufacturing (see Section D.1). Ongoing developments in experimental methods continue to expand the scope and applicability of mechanochemical processes in various scientific and industrial fields.

A.3. Theoretical approaches to mechanochemistry

Chemical reactions occur by collections of atoms (molecules or a solid) evolving from one metastable configuration (the reactants) on a multidimensional potential energy surface (PES) to another (the products) over an energy barrier. While there are, in principle, multiple pathways between the two states, the thermal process is dominated by the lowest-energy one by transiting a saddle point, which has an energy relative to the reactant, known as the activation energy. Mechanically induced processes, in particular, mechanochemistry, occur by imposed forces or stresses modifying the shape of this PES to change the heights of the energy barriers, ideally lowering them to cause the reaction rates to increase. An important potential advantage of mechanochemical processes is that they can, in principle, preferentially lower the energy of a higher barrier in the unmodified PES relative to the lowest-energy one to produce completely new products from those found in the thermal reaction.

The way the effects are calculated depends on whether the experiments control the stress (displacement) or the force (stress). In single-molecule activation (see Section A.1), where putatively well-defined pulling points are displaced, the change in energy barrier is computed using the COnstrained Geometries for simulating External Force (COGEF) method,[24] which distorts the reactant by displacing pulling points (PP) and by calculating the resulting change in energy *via* quantum mechanics.

However, it is more common to control the force, and the force/stress-modified PES yields a series of force-modified stationary points[25,26] that collectively define a so-called a Newton trajectory.[27] This allows the turning points (initial- and transition-states) on the modified PES to be calculated. In many experiments, the stresses modify the activation energies by a modest amount such that these theories that predict the forces at which the barriers decrease to zero are not necessary. In such cases, a perturbation method of transition-state theory[28] has been developed by Evans and Polanyi,[29] which assumes that the dominant effect of the force is to modify the equilibrium between the reactant and transition-state structures. This approach has proven effective in modeling surface[30] and bulk[31] mechanochemical reactions and understanding how the selectivity is modified.

B. Mechanochemical reactions across chemistry

B.1. Organic methods

A primary area in which mechanochemistry has made a significant impact is in organic chemistry. Under mechanochemical conditions, a wide range of organic reactions can be performed, resulting in higher yields, faster reactions, and more sustainable reaction conditions.[32–34] This is particularly important because the synthesis of complex organic molecules is a fundamental aspect of the pharmaceutical industry.[35] While many reactions have been successfully conducted under these conditions, there remains much to explore about how mechanochemistry can be applied to organic reactions.

The ability to synthesize complex molecules in the chemical industry relies heavily on a deep understanding of the mechanistic principles of organic chemistry. Traditional organic chemistry is deeply rooted in acid–base reactions and elimination–substitution chemistry. However, these concepts take on new significance in a solvent-free mechanochemical environment. Typically, organic chemists assess nucleophilicity and basicity based on the solvent, recognizing that reactivity changes depend on whether the medium is polar protic, polar aprotic, or non-polar. How does reactivity change when no solvent is present, and how can this be measured and controlled?

Moreover, solvents play a critical role in substitution reactions. For instance, in an S_N1 reaction, the first step involves forming a solvent-separated ion pair. Without a solvent, are S_N1 reactions feasible for mechanochemical reactions? Although there is an extensive library of reactions that can be conducted under mechanochemical conditions, it is essential to gain a deeper understanding of the mechanistic differences between traditional solvothermal reactions and mechanochemical ones. The key is to develop a better understanding of how these systems operate. Achieving this will allow mechanochemistry to have an even greater impact on the chemical community and society as a whole by offering new routes to sustainable chemical syntheses.

B.2. Mechanochemistry for inorganic materials and industrial applications

Inorganic materials, including metals, metal oxides, and ceramics, are ideal candidates for mechanochemical processing due to their robust physical properties. Mechanochemistry can be used to synthesize new materials, modify existing ones, and enhance their properties. Mechanochemical techniques can also modify the properties of inorganic materials. This includes enhancing their surface area, increasing porosity, and creating nanostructured materials. These modifications can improve the material's performance for various applications, such as catalysts, sensors, and battery electrodes.[36–38] Mechanochemical activation is particularly useful in catalysis, where it can enhance activity and selectivity.[39]

Mechanochemistry can be used to create advanced inorganic materials with tailored properties and includes the synthesis of nanomaterials, composites and hybrid materials. Mechanochemical processes can also be used to recycle waste materials, converting them into valuable products.[40]

Mechanochemistry can play a crucial role in developing energy-storage devices, such as batteries and supercapacitors, for example, to produce high-performance electrode materials, improve the conductivity of electrolytes and enhance the overall efficiency of energy-storage systems.[41]

It also offers environmentally friendly solutions for waste management and pollution control. This includes the degradation of hazardous substances, the immobilization of heavy metals, and the recycling of electronic waste.[42,43] Mechanochemical processes can significantly reduce the environmental impact of industrial activities.

The development of advanced mechanochemical equipment, such as high-energy ball mills and attritor mills, is crucial for the future developments. These tools can provide more precise control over the mechanical forces applied, leading to more consistent and reproducible results.

Mechanochemistry is increasingly being integrated with other technologies, such as microwave and ultrasound irradiation, to enhance its efficiency.[23] This combination of techniques can provide synergistic effects, opening new avenues for mechanochemical research and applications.

Mechanochemistry represents a powerful and versatile tool for synthesizing and modifying inorganic materials. Its application in various industries highlights its potential to revolutionize traditional chemical processes, offering environmentally friendly and efficient processes.

B.3. Polymers

Mechanochemistry has also opened new avenues in the areas of polymer degradation and recycling, smart materials development, and polymer synthesis. By enabling controlled chain scission, mechanochemistry reduces the polymer molecular weight and viscosity to facilitate more efficient recycling.[44,45] Smart polymer materials incorporate mechanophores that activate under stress or strain. These report on failure mechanisms in real-time or trigger material self-healing. In the area of polymer synthesis, mechanochemical techniques provide a solvent-free and energy-efficient way for sustainable materials production.[46]

The mechanical degradation of polymers was reported by Staudinger and coworkers in 1934.[47] Because polymer degradation posed a challenge for many applications, extensive research has focused on strategies to minimize this destructive process. Recent advances increasingly leverage mechanically induced bond scission in constructive ways to address pressing issues like plastic pollution. The main remediation strategies are the controlled depolymerization of custom-designed polymers with predetermined breaking points and the mechanical breakdown of common plastics in existing waste streams. For controlled depolymerization, force-responsive functionalities are strategically integrated into the polymer chains to ideally reform the original monomers. For plastic breakdown, ball milling has shown promise, for example, as demonstrated with polystyrene, where a significant drop in molecular weight, and even a measurable yield of styrene monomers, was achieved.[48] While further research is needed to understand the efficiency of depolymerization and breakdown in amorphous, crystalline and glassy regions, current advancements in molecular weight reduction may already help streamline existing chemical or emerging biological recycling processes that include plastic-degrading enzymes.

Mechanoresponsive molecular building blocks facilitate the development of smart polymer materials with self-reporting, self-healing or even self-reinforcing properties. Self-reporting capabilities often rely on the use of mechanochromic, mechanofluorescent or mechanoluminescent dyes, while other strategies include the activation of mechanocatalysis with optically detectable products, reactions of profluorescent molecules with mechanically generated radicals, supramolecular dye stacking and Förster resonance-energy transfer. Incorporated into the backbone or utilized as crosslinking units, these self-reporting capabilities have provided crucial insights into the mechanical failure mechanisms of polymers. Self-healing can generally be achieved by using reversible supramolecular or dynamic covalent bonds, but can also involve the activation of mechanocatalysts or the formation of mechanoradicals. Although mechanophores were initially applied primarily in thermoplastics and elastomers, recent advancements have extended their use to hydrogels. Mechanoresponsive and self-reporting hydrogels offer promising new applications in fields such as biomedicine and soft robotics, enabling innovations such as smart implants or adaptable, soft-robotic systems with built-in self-diagnostic and repair functions.

More recently, mechanochemistry has demonstrated significant potential for polymer synthesis where, for example, ball milling has been applied to chain-growth as well as step-growth polymerizations. Beyond linear homopolymers, mechanochemical methods have been used for creating block copolymers and for performing post-polymerization modifications. One example of the latter is the mechanochemical transformation of chitin into chitosan, where ball milling disrupted the crystalline structure, giving access to a larger number of functional groups and thus, ultimately, opening up novel routes for utilizing this abundant biopolymer.[49] Together, these developments highlight the potential of mechanochemistry to revolutionize polymer science, from sustainable production and recycling to the creation of multifunctional smart materials.

B.4. Mechanocatalysis

Mechanocatalysis is an emerging field that combines the principles of mechanochemistry and catalysis to modify reaction barriers and drive chemical reactions. Reactions such as Sonogashira,[50] Heck,[51] Suzuki,[52] and Negishi[53] and others have been successfully demonstrated under these unique conditions.[54] One of the key benefits of mechanocatalysis is its ability to facilitate reactions under ambient conditions, which is particularly useful for sensitive substrates that might degrade under high temperatures or harsh chemical environments.[55]

The future of the field lies in the application of direct mechanocatalysis.[56–58] Here, the milling jar and/or milling spheres themselves constitute the catalytic material that drives the reaction. This approach has been demonstrated for various reactions and, similar to other forms of mechanocatalysis using traditional catalysts, direct mechanocatalytic reactions are impactful due to their ease of use and low cost of reagents. Additionally, direct mechanocatalysis can enable unique reaction pathways that are not accessible through conventional methods.[59]

The progress of this field will depend on the ability to recycle the catalytic material, especially if it is a precious metal such as palladium or platinum. In the pharmaceutical industry, the ability to remove the metal from active pharmaceutical ingredients is also an important aspect.[60]

B.5. Supramolecular materials

The combination of mechanochemistry and supramolecular chemistry[61] opens exciting new opportunities for developing new functional materials, for improved and more efficient chemical synthesis and catalysis,[62] as well as for the isolation of increasingly complex structures as bulk materials. The efficiency of syntheses using milling, grinding, extrusion or other techniques has made mechanochemistry a highly popular technique to discover, as well as to synthesise new pharmaceutical materials, such as hydrogen-bonded cocrystals or polymorphs. This is possible even using continuous twin-screw extrusion.[63] This, and other reactors such as drum and vibrating eccentric mills are leading to new, efficient, and scalable approaches to manufacture pharmaceutical materials.[64,65] Future translation of such benefits towards other, more exotic and complex, functional self-assembled materials, such as semiconductor cocrystals,[66] catenanes or rotaxanes,[67] will, for the first time, make such systems accessible in bulk for the development of new technologies.

Mechanochemistry also offers a means to advance the fundamental understanding of supramolecular interactions, by permitting more efficient, real-time exploration of molecular recognition processes in the absence of competing solvents. Learning how to combine reversible covalent bond formation with mechanochemistry[68] will enable the manipulation of reaction equilibria for improved reaction efficiency, the synthesis of novel (supra) molecular architectures *via* dynamic covalent chemistry in a solventless environment, or the more efficient production of such structures.[69] Finally, real-time monitoring of mechanochemical reactions has led to the identification of cocrystals as reactive, solid-state intermediates in a number of covalent bond-forming reactions.[70] While such cocrystals provide insights into molecular-assembly processes under mechanochemical conditions, they will also present blueprints for designing supramolecular surrogates for reagents that are difficult to synthesize and store.[71]

C. Mechanochemical processes in living systems

C.1. Mechanochemical and chemomechanical signal conversion in biology

Mechanical forces play important roles in biology. Biological systems have evolved to address a diverse range of mechanical challenges, including materials with exceptional strength and toughness as well as those that strengthen under load. Mechanochemical reactions enable biological systems to sense mechanical signals and to adapt to changes in their mechanical environment (mechanosensing and mechanotransduction). Key players in these processes are proteins that respond to tensile, compressive or shear forces by undergoing specific conformational changes. They can form catch bonds (bonds that strengthen under load), expose cryptic binding or catalytic sites, or become susceptible to cleavage. These mechanisms are mimicked in synthetic systems, such as catch bonds based on DNA nanotechnology[72,73] and mechanically activated catalysts (see Section B.4)[74] In addition to mechanosensors, biology has also evolved molecular motors and actuation systems that convert chemical energy into lateral or rotational displacements, allowing cells and organisms to move and change shape. These biological strategies and mechanisms inspire the field of polymer mechanochemistry (see Section B.3) and pave the way for the design of biomimetic smart materials capable of adaptive, self-healing or force-responsive behaviors.

C.2. Targeting biological questions with mechanochemistry

Mechanobiology and mechanochemistry share many mechanical characterization methods, from the single-molecule to the bulk material scale. Mechanochemistry further provides mechanophores, mechanoresponsive polymers and smart materials for interfering with biological systems. Mechanophores that respond to cell-generated forces in 2D or 3D cellular environments may serve as diagnostic tools to identify and characterize cells with altered mechanical responses, which are common in a range of diseases (*e.g.*, cancer, atherosclerosis, asthma, fibrosis). Mechanically tailored biomaterials may serve as synthetic extracellular matrix mimics to influence cell responses in regenerative medicine, while mechano-activated drug delivery systems are also being developed. Emerging drug delivery strategies envision using ultrasound to release small molecules from polymers with latent mechanophores[75] and leveraging cell-generated forces *in situ* to trigger drug release and uptake.[76] Overall, the interaction between mechanochemistry and mechanobiology is an exciting frontier, offering innovative approaches for diagnostics, therapeutics or tissue engineering, with potential to reshape how we address diseases linked to altered cell mechanics.

D. Applications of mechanochemistry

D.1. Green chemistry and solvent-free syntheses

Integrating mechanochemistry into green-chemistry practices holds significant potential for the pharmaceutical industry, materials science, and other fields that rely heavily on chemical syntheses. Based on the twelve principles of Green Chemistry, mechanochemistry can directly address and contribute to more than half of them.[77–80] Mechanochemical reactions have been shown to prevent waste, significantly reduce solvent use, be catalytic, be less hazardous, reduce energy consumption, use safer chemicals, and minimize derivatives. Since solvents contribute significantly to chemical waste, especially in the chemical industry, reducing their use alone is a huge benefit in developing sustainable chemical practices.[81,82]

To further enhance the synergy between green chemistry and mechanochemistry, sustainable goals must be developed specifically for mechanochemistry to foster innovative technologies that are both economically viable and environmentally benign. While mechanochemistry can significantly impact green chemistry simply by reducing solvent use, many other principles are often overlooked. The field of mechanochemistry has the potential to develop reactions that fully incorporate all 12 principles, but there needs to be a focus on principles other than solvent reduction.

As industries and researchers continue to seek sustainable solutions to chemical synthetic problems, the importance of green chemistry and mechanochemistry will only grow, driving the transition to more sustainable practices and contributing to a healthier planet.

D.2. Mechanochemical processing for pharmaceuticals

Mechanochemistry has also emerged as a transformative approach for the synthesis of active pharmaceutical ingredients (APIs),[83–85] offering significant advantages over traditional synthetic techniques, particularly in terms of sustainability, efficiency, and product optimization.

The pharmaceutical industry's growing emphasis on green chemistry and sustainable manufacturing practices places mechanochemistry in a privileged position for API development. The possibility of minimising or completely eliminating organic solvents, which are often associated with environmental hazards and high production costs, overcomes the solvent waste issue (see Section D.1).[86] Additionally, enabling cleaner processes that generate fewer byproducts and reduce waste, mechanochemical processes address both economic and environmental challenges, which makes them a vital tool for advancing pharmaceutical innovation and sustainability.

Seminal examples have demonstrated that both batch[87] and continuous-flow mechanochemistry[17] are suitable for the scalability of World Health Organisation (WHO) essential medicines or pharmaceutical co-crystals,[64] with improved green chemistry[88] and environmental metrics[82] compared to the corresponding manufacturing processes in solution.

Additionally, mechanochemistry enables the design of APIs with improved physical and chemical properties. For instance, it facilitates the production of co-crystals, amorphous materials, and nano-sized particles, which can enhance the solubility, stability, and bioavailability of pharmaceuticals, which are crucial for improving drug efficacy and patient outcomes, especially for poorly soluble compounds. Mechanochemical processes also allow new molecules and reactivities to be achieved that would otherwise be impossible in solution,[89] and potentially tailoring API production to specific needs.

D.3. Low-technology industrial processes

As the industrial revolution started in the 18th century, new industries grew over a period of decades, along with development of the requisite supporting infrastructure of roads, railways and canals. This allowed a limited number of large facilities to efficiently make products that could then be transported to where they were needed through a sophisticated worldwide transportation network. This model has worked (reasonably) well for advanced industrial nations, but less well for developing countries, because it is difficult for poorer countries to develop the requisite infrastructure to get their feet onto the first rungs of the industrial development ladder. New technologies have helped developing countries develop alternative approaches to those used in developed ones; a recent example in the area of finance has been the use of cheap and simple cellphones to build an alternative payment and banking system in Africa. In a similar way to which new technologies might be built in new settlements in space (see Section E.1), mechanochemical syntheses could provide local technologies that do not require large complex equipment. One example is the local mechanocatalytic synthesis of fertilizers (see Section B.4),[90,91] which could be made locally and close to the location where they will be used. Mechanochemical synthesis of pharmaceuticals (Section D.2) not only requires less solvent to provide environmentally more acceptable synthetic methods, but it is also simpler.

D.4. Mechanical materials processing

Mechanochemistry has a long history of being used to process and modify materials, largely beginning in the areas of metals and inorganic materials.[92] An additional area that mechanochemistry is seeing a marked impact in is the processing of materials, for re-activating and recycling of materials, providing greener and more sustainable approaches to these processes for upcycling. Examples include the breakdown[93] and conversion of poly(ethylene terephthalate) (PET) into metal–organic frameworks (MOFs)[94] where the mechanical milling of PETs affords their degradation which, when combined with the appropriate metal ions, enables the direct formation of MOFs. Interestingly, MOFs formed under mechanochemical conditions, such as liquid-assisted grinding, were shown to exhibit a highly dynamic character, demonstrating increased solubilities, and an ability to readily interconvert between materials of different structure, topology and dimensionality.[95] Such observations highlight mechanical treatment as a means to transform, assemble, or even disassemble, otherwise robust materials. Such approaches have also shown that MOFs can be completely reconstructed under mechanical milling, affording new modalities of materials design through phase transformations.[96] The extraction of biomaterials has also been enabled by mechanochemistry, with the isolation of materials such as chitin from waste crab shells,[97] demonstrating how such approaches can be used for more sustainable production of this important material, with additional studies elucidating how the chitin can be further processed mechanochemically into chitosan with controlled molecular weight.[98]

D.5. Tribochemistry

Tribochemistry, from the Greek “to rub”, is broadly defined as the study of contacting bodies in relative motion and encompasses effects such as friction, wear and lubrication. In general, it describes processes that are induced by a combination of normal and shear stresses and the field is viewed as a subfield of mechanical engineering. As first pointed out by Jost in the 1950's, a significant proportion of the gross-domestic product of an industrialized nation is lost due to friction, wear and the failure of mechanical components. More recently, it was realized that such losses also contribute to greenhouse gas emissions, so that the design of new, friction- and wear-reducing lubricants will contribute to mitigating the emission of greenhouses gases.[99] As a result, tribochemistry is arguably the most currently economically important field of mechanochemistry.

Early research to understand tribochemistry invoked an array of effects from high local temperatures at contacting asperities in the sliding interface to the creation of plasmas that induced reactions. However, over the last few years, it was realized that additives to lubricants that form friction- and wear-reducing films could react under mild siding conditions through mechanochemical reaction pathways.[100–102] Under more severe, extreme-pressure lubrication regimes, the reactivity is dominated by the high interfacial temperatures.[103,104]

Common general principles underpin both tribochemistry and mechanochemistry; that is, applied forces/stresses modify the potential energy profile of the system to modify, and ideally lower, the energy barrier to increase the rate of the process. This notion was first proposed in the 1920's by Prandtl[105] by using a simple sinusoidal potential with the goal of analyzing the non-elastic behavior of materials, but it was subsequently realized that this approach could also be used to describe friction and the model has been verified for the sliding of an atomic force microscope tip over a surface in numerous situations. A similar general approach of using transition-state theory with a sinusoidal potential energy was used by Eyring to develop a molecular-scale model of viscosity.[106] These friction, viscosity and mechanochemical models therefore depend on a common physical principle and work to understand tribochemical processes will inform our understanding of mechanochemistry, and *vice versa*.

E. Future directions

E.1. A role for mechanochemistry in space?

Potential new directions for mechanochemistry also include its use in space exploration. Central to the needs for manned missions on the Moon or Mars are the ability to generate resources, such as oxygen and water that will be essential for long-duration missions. While there are numerous approaches that have been proposed for the use of regolith as the source for generating these, much of the focus has been around using electrochemical processes.[107–109] One can envision how mechanochemical processes could be used to take advantage of regolith in order to also generate important reactants such as perchlorates and nitrates.[110] Such opportunities for *in situ* resource utilization are already envisioned for lunar construction,[111] but, due to mechanochemical syntheses being largely solvent free, this also opens the door to using locally sourced materials for chemical manufacturing as well. With regolith being rich in transition metals,[112,113] these sources represent natural materials from which catalyst systems can be made, which could then be used for oxygen and water reclamation.

E.2. Mechanochemistry, digitalization, and robotics

Mechanochemistry, digitalisation, and robotics represent three pivotal realms of contemporary science and technology. Each domain holds significant promise, yet their convergence opens up unprecedented opportunities for innovation and advancement and their intersection holds immense potential for advancing scientific research and industrial applications. By integrating these fields, researchers can create more efficient, precise, and scalable processes. Some potential examples are outlined below.

Robotics can be employed to automate mechanochemical syntheses, ensuring the consistent application of mechanical force and precise control over reaction conditions. Digitalisation can further enhance these processes by enabling real-time monitoring and analysis of reactions, providing immediate feedback to allow rapid optimization.

The integration of big data, machine learning and artificial intelligence (AI) methods with mechanochemistry can lead to a deeper understanding of reaction mechanisms and the discovery of new reactions. By analysing large datasets generated from mechanochemical experiments, AI algorithms can identify patterns and predict optimal reaction conditions, accelerating the development of new materials and compounds.

One of the major challenges for mechanochemical syntheses is ensuring the reproducibility of results. Robotics and digitalisation can address this issue by standardizing experimental procedures and providing detailed documentation of each step. This not only enhances reproducibility but also facilitates the scaling up of mechanochemical processes for industrial applications.

Several case studies have highlighted the successful integration of mechanochemistry, digitalisation, and robotics, for example, in the areas of sustainable chemistry; the combination of robotics and digitalisation has allowed the development of sustainable mechanochemical processes that are both efficient and environmentally friendly.[114]

While the integration of mechanochemistry, digitalisation and robotics holds great promise, several challenges remain. Ensuring the compatibility of different systems and technologies, managing large volumes of data, and addressing the high costs associated with advanced robotics are some of the hurdles that need to be overcome.

Future research will focus on developing sophisticated robotic systems that can handle a wide range of mechanochemical reactions, as well as creating comprehensive digital platforms that can seamlessly integrate data from different sources. Additionally, fostering interdisciplinary collaborations will be crucial to address these challenges and to unlock the full potential of these technologies.

The convergence of mechanochemistry, digitalization, and robotics represents a transformative force in modern science. By leveraging the strengths of each field, researchers can achieve unprecedented levels of efficiency, precision, and innovation.

E.3. A merging of areas for greener chemistry – mechanochemistry and electrification of the chemical industry

In an effort to decarbonize the chemical industry, electrification of industrial processes provides a means to aid in the reduction of greenhouse gas emissions.[115–117] While numerous approaches are under consideration, the adoption of mechanochemical methods affords one direct option that has received little attention. If one considers the majority of mechanochemical reactors, they are already immediately implementable using renewables to power them. Key reactions such as ammonia synthesis, which normally requires high temperatures and pressures, have been shown to occur mechanochemically at lower temperatures and pressures than the thermal procees.[90,118] This demonstration opens the door for the adaptation of other such large-scale syntheses to mechanochemical approaches. While there is still a long way to go, the design and translation of other reaction platforms to mechanochemical methods could enable a marked reduction in the energy needs and greenhouse-gas emissions of industry.[88]

References

1 H. J. Theophrastus, *Theophrastus's History of Stones : with an English Version, and Critical and Philosophical Notes, Including the Modern History of the Gems, &c., Described by that Author, and of Many Other of the Native Fossils*, London, 1774.

2 M. Faraday, *Chemical Manipulation: Being Instructions to Students in Chemistry on the Methods of Performing Experiments of Demonstration or of Research with Accuracy and Success*, Carey and Lea, Philadelphia, 1831.

3 W. C. Röntgen, *Ann. Phys.*, 1892, **281**, 98–107.

4 Y. Liu, S. Holm, J. Meisner, Y. Jia, Q. Wu, T. J. Woods, T. J. Martinez and J. S. Moore, *Science*, 2021, **373**, 208–212.

5 Y. Sun, F. Xie and J. S. Moore, *J. Am. Chem. Soc.*, 2024, **146**, 31702–31714.

6 B. Chen, R. Hoffmann and R. Cammi, *Angew. Chem., Int. Ed.*, 2017, **56**, 11126–11142.

7 S. Lüdtke, P. Neumann, K. M. Erixon, F. Leeper, R. Kluger, R. Ficner and K. Tittmann, *Nat. Chem.*, 2013, **5**, 762–767.

8 R. Rana, G. Djuidje Kenmoe, F. Sidoroff, R. Bavisotto, N. Hopper and W. T. Tysoe, *J. Phys. Chem. C*, 2022, **126**, 11585–11593.

9 N. Hopper, F. Sidoroff, J. Cayer-Barrioz, D. Mazuyer and W. T. Tysoe, *Tribol. Lett.*, 2023, **71**, 121.

10 M. Zhang, R. Nixon, F. Schaufelberger, L. Pirvu, G. De Bo and D. A. Leigh, *Nat. Chem.*, 2024, **16**, 1366–1372.

11 L. Chen, R. Nixon and G. De Bo, *Nature*, 2024, **628**, 320–325.

12 J.-L. Do and T. Friščić, *ACS Cent. Sci.*, 2017, **3**, 13–19.

13 P. Baláž, M. Achimovičová, M. Baláž, P. Billik, Z. Cherkezova-Zheleva, J. M. Criado, F. Delogu, E. Dutková, E. Gaffet, F. J. Gotor, R. Kumar,

I. Mitov, T. Rojac, M. Senna, A. Streletskii and K. Wieczorek-Ciurowa, *Chem. Soc. Rev.*, 2013, **42**, 7571–7637.
14 A. A. L. Michalchuk, E. V. Boldyreva, A. M. Belenguer, F. Emmerling and V. V. Boldyrev, *Front. Chem.*, 2021, **9**, 685789.
15 A. A. L. Michalchuk, A. Kabelitz and F. Emmerling, in *Nontraditional Activation Methods in Green and Sustainable Applications*, ed. B. Török and C. Schäfer, Elsevier, 2021, pp. 369–419.
16 D. E. Crawford, C. K. G. Miskimmin, A. B. Albadarin, G. Walker and S. L. James, *Green Chem.*, 2017, **19**, 1507–1518.
17 D. E. Crawford, A. Porcheddu, A. S. McCalmont, F. Delogu, S. L. James and E. Colacino, *ACS Sustain. Chem. Eng.*, 2020, **8**, 12230–12238.
18 A. A. L. Michalchuk, K. S. Hope, S. R. Kennedy, M. V. Blanco, E. V. Boldyreva and C. R. Pulham, *Chem. Commun.*, 2018, **54**, 4033–4036.
19 C. B. Lennox, T. H. Borchers, L. Gonnet, C. J. Barrett, S. G. Koenig, K. Nagapudi and T. Friščić, *Chem. Sci.*, 2023, **14**, 7475–7481.
20 O. Galant, G. Cerfeda, A. S. McCalmont, S. L. James, A. Porcheddu, F. Delogu, D. E. Crawford, E. Colacino and S. Spatari, *ACS Sustain. Chem. Eng.*, 2022, **10**, 1430–1439.
21 N. Y. Gugin, J. A. Villajos, O. Dautain, M. Maiwald and F. Emmerling, *ACS Sustain. Chem. Eng.*, 2023, **11**, 5175–5183.
22 N. Y. Gugin, K. V. Yusenko, A. King, K. Meyer, D. Al-Sabbagh, J. A. Villajos and F. Emmerling, *Chem*, 2024, **10**, 3459–3473.
23 V. Martinez, T. Stolar, B. Karadeniz, I. Brekalo and K. Užarević, *Nat. Rev. Chem*, 2023, **7**, 51–65.
24 M. K. Beyer, *J. Chem. Phys.*, 2000, **112**, 7307–7312.
25 G. Subramanian, N. Mathew and J. Leiding, *J. Chem. Phys.*, 2015, **143**, 134109.
26 S. K. Jha, K. Brown, G. Todde and G. Subramanian, *J. Chem. Phys.*, 2016, **145**, 074307.
27 W. Quapp, J. M. Bofill and J. Ribas-Ariño, *Int. J. Quantum Chem.*, 2018, **118**, e25775.
28 H. Eyring, *J. Chem. Phys.*, 1935, **3**, 107–115.
29 M. G. Evans and M. Polanyi, *Trans. Faraday Soc.*, 1935, **31**, 875–894.
30 N. Hopper, F. Sidoroff, R. Rana, R. Bavisotto, J. Cayer-Barrioz, D. Mazuyer and W. T. Tysoe, *Phys. Chem. Chem. Phys.*, 2023, **25**, 15855–15861.
31 N. Hopper, F. Sidoroff, J. Cayer-Barrioz, D. Mazuyer, B. Chen and W. T. Tysoe, *RSC Mechanochem.*, 2024, **1**, 402–412.
32 J. F. Reynes, F. Leon and F. García, *ACS Org. Inorg. Au*, 2024, **4**, 432–470.
33 J. Andersen and J. Mack, *Green Chem.*, 2018, **20**, 1435–1443.
34 D. Tan and T. Friščić, *Eur. J. Org. Chem.*, 2018, 18–33.
35 D. C. Blakemore, L. Castro, I. Churcher, D. C. Rees, A. W. Thomas, D. M. Wilson and A. Wood, *Nat. Chem.*, 2018, **10**, 383–394.
36 G. A. A. Bazedi, A. E. Al-Rawajfeh, M. A. Abdel-Fatah, M. R. Alrbaihat and E. AlShamaileh, in *Handbook of Greener Synthesis of Nanomaterials and Compounds*, ed. B. Kharisov and O. Kharissova, Elsevier, 2021, pp. 405–418.
37 A. Scano and G. Ennas, in *A Practical Introduction from Soft to Hard Materials*, ed. E. Colacino, G. Ennas, I. Halasz, A. Porcheddu and A. Scano, De Gruyter, 2021, pp. 23–40.
38 Z. Hong, D. Tan, R. A. John, Y. K. E. Tay, Y. K. T. Ho, X. Zhao, T. C. Sum, N. Mathews, F. García and H. S. Soo, *iScience*, 2019, **16**, 312–325.
39 S. L. James, C. J. Adams, C. Bolm, D. Braga, P. Collier, T. Friscic, F. Grepioni, K. D. M. Harris, G. Hyett, W. Jones, A. Krebs, J. Mack, L. Maini, A. G. Orpen, I. P. Parkin, W. C. Shearouse, J. W. Steed and D. C. Waddell, *Chem. Soc. Rev.*, 2012, **41**, 413–447.
40 T. Auvray and T. Friščić, *Molecules*, 2023, **28**, 897.
41 Z. Chen, G.-F. Han, A. Mahmood, J. Hou, W. Wei, H. Kyong Shon, G. Wang, T. David Waite, J.-B. Baek and B.-J. Ni, *Prog. Mater. Sci.*, 2024, **145**, 101299.
42 Y. Jiang, X. Chen, S. Yan, Y. Ou and T. Zhou, *Green Chem.*, 2022, **24**, 5987–5997.
43 O. Dolotko, N. Gehrke, T. Malliaridou, R. Sieweck, L. Herrmann, B. Huzinger, M. Knapp and H. Ehrenberg, *Commun. Chem.*, 2023, **6**, 49.
44 S. Aydonat, A. H. Hergesell, C. L. Seitzinger, R. Lennarz, G. Chang, C. Sievers, J. Meisner, I. Vollmer and R. Göstl, *Polym. J.*, 2024, **56**, 249–268.
45 J. Zhou, T.-G. Hsu and J. Wang, *Angew. Chem., Int. Ed.*, 2023, **62**, e202300768.
46 A. Krusenbaum, S. Grätz, G. T. Tigineh, L. Borchardt and J. G. Kim, *Chem. Soc. Rev.*, 2022, **51**, 2873–2905.
47 H. Staudinger and W. Heuer, *Ber. Dtsch. Chem. Ges.*, 1934, **67**, 1159–1164.
48 V. P. Balema, I. Z. Hlova, S. L. Carnahan, M. Seyedi, O. Dolotko, A. J. Rossini and I. Luzinov, *New J. Chem.*, 2021, **45**, 2935–2938.
49 T. Di Nardo, C. Hadad, A. Nguyen Van Nhien and A. Moores, *Green Chem.*, 2019, **21**, 3276–3285.
50 R. Thorwirth, A. Stolle and B. Ondruschka, *Green Chem.*, 2010, **12**, 985–991.
51 J. Yu, H. Shou, W. Yu, H. Chen and W. Su, *Adv. Synth. Catal.*, 2019, **361**, 5133–5139.
52 T. Seo, T. Ishiyama, K. Kubota and H. Ito, *Chem. Sci.*, 2019, **10**, 8202.
53 Q. Cao, J. L. Howard, E. Wheatley and D. L. Browne, *Angew Chem. Int. Ed. Engl.*, 2018, **57**, 11339–11343.
54 K. Kubota and H. Ito, *Trends Chem.*, 2020, **2**, 1066.
55 K. Kubota, R. Takahashi and H. Ito, *Chem. Sci.*, 2019, **10**, 5837–5842.
56 S. Hwang, S. Grätz and L. Borchardt, *Chem. Commun.*, 2022, **58**, 1661–1671.
57 W. Pickhardt, C. Beaković, M. Mayer, M. Wohlgemuth, F. J. L. Kraus, M. Etter, S. Grätz and L. Borchardt, *Angew Chem. Int. Ed. Engl.*, 2022, **61**, e202205003.
58 R. A. Haley, A. R. Zellner, J. A. Krause, H. Guan and J. Mack, *ACS Sustainable Chem. Eng.*, 2016, **4**, 2464–2469.

59 R. A. Haley, J. Mack and H. Guan, *Inorg. Chem. Front.*, 2017, **4**, 52–55.
60 M. Economidou, N. Mistry, K. M. P. Wheelhouse and D. M. Lindsay, *Org. Process Res. Dev.*, 2023, **27**, 1585–1615.
61 A. Bose and P. Mal, *Beilstein J. Org. Chem.*, 2019, **15**, 881–900.
62 S. P. Yelgaonkar, D. C. Swenson and L. R. MacGillivray, *Chem. Sci.*, 2020, **11**, 3569–3573.
63 D. Daurio, K. Nagapudi, L. Li, P. Quan and F.-A. Nunez, *Faraday Discuss.*, 2014, **170**, 235–249.
64 A. Bodach, A. Portet, F. Winkelmann, B. Herrmann, F. Gallou, E. Ponnusamy, D. Virieux, E. Colacino and M. Felderhoff, *ChemSusChem*, 2024, **17**, e202301220.
65 J.-H. Schöbel, F. Winkelmann, J. Bickera and M. Felderhoff, *RSC Mechanochem.*, 2025, DOI: 10.1039/D4MR00096J.
66 H. T. Black and D. F. Perepichka, *Angew Chem. Int. Ed. Engl.*, 2014, **53**, 2138–2142.
67 M. Holler, T. Stoerkler, A. Louis, F. Fischer and J.-F. Nierengarten, *Eur. J. Org Chem.*, 2019, **2019**, 3401–3405.
68 T. E. Shaw, J. Arami, J.-F. Ayme, J.-M. Lehn and T. Jurca, *RSC Mechanochem.*, 2024, **1**, 33–37.
69 M. Pascu, A. Ruggi, R. Scopelliti and K. Severin, *Chem. Commun.*, 2013, **49**, 45–47.
70 K. J. Ardila-Fierro and J. G. Hernández, *Angew. Chem., Int. Ed.*, 2024, **63**, e202317638.
71 J. M. Marrett, H. M. Titi, Y. Teoh and T. Friščić, *Chem. Sci.*, 2024, **15**, 298–306.
72 M. van Galen, A. Bok, T. Peshkovsky, J. van der Gucht, B. Albada and J. Sprakel, *Nat. Chem.*, 2024, **16**, 1943–1950.
73 M. Yang, D. T. R. Bakker and I. T. S. Li, *Nat. Commun.*, 2024, **15**, 8828.
74 A. Piermattei, S. Karthikeyan and R. P. Sijbesma, *Nat. Chem.*, 2009, **1**, 133–137.
75 S. Huo, P. Zhao, Z. Shi, M. Zou, X. Yang, E. Warszawik, M. Loznik, R. Göstl and A. Herrmann, *Nat. Chem.*, 2021, **13**, 131–139.
76 A. Velusamy, R. Sharma, S. A. Rashid, H. Ogasawara and K. Salaita, *Nat. Commun.*, 2024, **15**, 704.
77 J. F. Reynes, V. Isoni and F. García, *Angew Chem. Int. Ed. Engl.*, 2023, **62**, e202300819.
78 E. Colacino, V. Isoni, D. E. Crawford and F. García, *Trends Chem.*, 2021, **3**, 335–339.
79 P. Sharma, C. Vetter, E. Ponnusamy and E. Colacino, *ACS Sustainable Chem. Eng.*, 2022, **10**, 5110–5116.
80 N. Fantozzi, J.-N. Volle, A. Porcheddu, D. Virieux, F. García and E. Colacino, *Chem. Soc. Rev.*, 2023, **52**, 6680–6714.
81 R. A. Sheldon, *Green Chem.*, 2017, **19**, 18–43.
82 O. Galant, G. Cerfeda, A. S. McCalmont, S. L. James, A. Porcheddu, F. Delogu, D. E. Crawford, E. Colacino and S. Spatari, *ACS Sustainable Chem. Eng.*, 2022, **10**, 1430–1439.
83 E. Colacino, A. Porcheddu, C. Charnay and F. Delogu, *React. Chem. Eng.*, 2019, **4**, 1179–1188.
84 M. Pérez-Venegas and E. Juaristi, *ACS Sustain. Chem. Eng.*, 2020, **8**, 8881–8893.
85 P. Ying, J. Yu and W. Su, *Adv. Synth. Catal.*, 2021, **363**, 1246–1271.
86 M. J. Raymond, C. S. Slater and M. J. Savelski, *Green Chem.*, 2010, **12**, 1826–1834.
87 R. Geib, E. Colacino and L. Gremaud, *ChemSusChem*, 2024, **17**, e202301921.
88 N. Fantozzi, J.-N. Volle, A. Porcheddu, D. Virieux, F. García and E. Colacino, *Chem. Soc. Rev.*, 2023, **52**, 6680–6714.
89 A. Porcheddu, F. Cuccu, L. De Luca, F. Delogu, E. Colacino, N. Solin and R. Mocci, *ChemSusChem*, 2022, **15**, e202200362.
90 G.-F. Han, F. Li, Z.-W. Chen, C. Coppex, S.-J. Kim, H.-J. Noh, Z. Fu, Y. Lu, C. V. Singh, S. Siahrostami, Q. Jiang and J.-B. Baek, *Nat. Nanotechnol.*, 2021, **16**, 325–330.
91 F. Cuccu, D. L. Browne and A. Porcheddu, *ChemCatChem*, 2023, **15**, e202300762.
92 C. Suryanarayana, *Prog. Mater. Sci.*, 2001, **46**, 1–184.
93 V. Štrukil, *ChemSusChem*, 2021, **14**, 330–338.
94 P. He, Z. Hu, Z. Dai, H. Bai, Z. Fan, R. Niu, J. Gong, Q. Zhao and T. Tang, *ChemSusChem*, 2023, **16**, e202201935.
95 W. Yuan, T. Friščić, D. Apperley and S. L. James, *Angew. Chem., Int. Ed.*, 2010, **49**, 3916–3919.
96 H. K. Lee, J. H. Lee and H. R. Moon, *Inorg. Chem.*, 2021, **60**, 11825–11829.
97 F. Hajiali, J. Vidal, T. Jin, L. C. de la Garza, M. Santos, G. Yang and A. Moores, *ACS Sustain. Chem. Eng.*, 2022, **10**, 11348–11357.
98 G. Yang, E. Lam and A. Moores, *ACS Sustain. Chem. Eng.*, 2023, **11**, 7765–7774.
99 K. Holmberg, P. Andersson and A. Erdemir, *Tribol. Int.*, 2012, **47**, 221–234.
100 N. N. Gosvami, J. A. Bares, F. Mangolini, A. R. Konicek, D. G. Yablon and R. W. Carpick, *Science*, 2015, **348**, 102–106.
101 J. R. Felts, A. J. Oyer, S. C. Hernández, K. E. Whitener Jr, J. T. Robinson, S. G. Walton and P. E. Sheehan, *Nat. Commun.*, 2015, **6**, 6467.
102 A. Boscoboinik, D. Olson, H. Adams, N. Hopper and W. T. Tysoe, *Chem. Commun.*, 2020, **56**, 7730–7733.
103 P. V. Kotvis and W. T. Tysoe, *Tribol. Trans.*, 1998, **41**, 117–123.
104 T. J. Blunt, P. V. Kotvis and W. T. Tysoe, *Tribol. Trans.*, 1998, **41**, 129–139.
105 L. Prandtl and Z. Angew, *Math. Mech.*, 1928, **8**, 85.
106 W. Kauzmann and H. Eyring, *J. Am. Chem. Soc.*, 1940, **62**, 3113–3125.
107 A. Meurisse, B. Lomax, Á. Selmeci, M. Conti, R. Lindner, A. Makaya, M. D. Symes and J. Carpenter, *Planet. Space Sci.*, 2022, **211**, 105408.
108 L. Schlüter, A. Cowley, Y. Pennec and M. Roux, *Acta Astronaut.*, 2021, **179**, 371–381.
109 Anita, J. W. Bullard and S. Banerjee, *Trends Chem.*, 2022, **4**, 260–263.
110 J. O. Edgar, J. A. Gould, K. Badreshany and J. Telling, *Icarus*, 2022, **387**, 115202.
111 N. I. Cool, S. Perez-Beltran, J. Cheng, N. Rivera-Gonzalez, D. Bronner, Anita, E. Wang, U. Zakira, M. Farahbakhsh, K.-W. Liu, J.-L. Hsu, B. Birgisson and S. Banerjee, *iScience*, 2023, **26**, 106382.
112 G. A. Landis, *Acta Astronaut.*, 2007, **60**, 906–915.
113 J. N. Rasera, J. J. Cilliers, J. A. Lamamy and K. Hadler, *Planet. Space Sci.*, 2020, **186**, 104879.

114 Y. Nakajima, K. Kawasaki, Y. Takeichi, M. Hamaya, Y. Ushiku and K. Ono, *Digital Discovery*, 2024, **3**, 2130–2136.
115 J. L. Barton, *Science*, 2020, **368**, 1181–1182.
116 Z. J. Schiffer and K. Manthiram, *Joule*, 2017, **1**, 10–14.
117 D. S. Mallapragada, Y. Dvorkin, M. A. Modestino, D. V. Esposito, W. A. Smith, B.-M. Hodge, M. P. Harold, V. M. Donnelly, A. Nuz, C. Bloomquist, K. Baker, L. C. Grabow, Y. Yan, N. N. Rajput, R. L. Hartman, E. J. Biddinger, E. S. Aydil and A. D. Taylor, *Joule*, 2023, **7**, 23–41.
118 S. Reichle, M. Felderhoff and F. Schüth, *Angew. Chem., Int. Ed.*, 2021, **60**, 26385–26389.