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# Moving mechanochemistry forward: mechanocatalysis

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Mechanocatalysis is an exciting subfield of mechanochemistry, although it is still relatively young. Web of Science searches for relevant descriptors (*mechanocatal** or *mechano-catal** or *tribocatal** or *tribo-catal**) reveal a few scattered publications after 1994. A strong increase started around 2013 so that about 100 articles were published in 2025, many of them in *RSC Mechanochemistry*.

Since there is not yet any generally accepted definition of "mechanocatalysis", the term is often used rather loosely. The mere enhancement of reaction rates by the influence of mechanical forces is one of the hallmarks of mechanochemistry as a whole and thus is not useful as the basis of a definition.

As such, we look to take this opportunity to propose the following definition and welcome comments from the mechanochemistry and mechanocatalysis community.

"*Mechanocatalysis is any reaction, which is catalyzed – be it by a solid surface or a molecular entity – without the influence of mechanical forces, but for which rates or reaction pathways are then altered when the system is mechanically agitated*".

Mechanochemistry is also very relevant to the synthesis of catalytic materials themselves, as many catalytically interesting materials can be prepared by ball milling and related techniques,[1] but we would not refer to this process of mechanical catalyst generation as mechanocatalysis.

Despite the relatively short time during which mechanocatalysis has been studied, the synthetic scope covered by this subfield has been shown to be rather broad. The approach is well established in the fields of homogeneous catalysis, such as in Heck- or Suzuki-reactions,[2] in organocatalysis,[3] in heterogeneously catalyzed gas-phase reactions,[4,5] and it is expected that the discovery of additional reactions and new phenomena will continue. Particularly interesting is the development of so-called *direct mechanocatalysis*,[6] in which the materials of balls and milling vessel themselves are made from catalytically active materials that further increase the activity by milling.[7–9]

Mechanocatalysis is especially intriguing because the underlying reasons for enhanced catalytic reactivity are largely unexplored. Various mechanistic reasons have been invoked, and in some cases, experimental support has been given. For the deconstruction of polyolefins, mechanogenerated radicals have been detected and proven to be important.[10–12] Radicals were also found to be relevant to the monochlorination of methane.[13] Other suggested sources of increased activity, such as hot spots during collision of balls,[14] still need to be experimentally validated or theoretically calculated. The creation of mechanically induced, short-lived, high activity defects in the catalyst (for example as shown by Blair *et al.* for hexagonal boron nitride[15]), the continuous generation of fresh surfaces,[16] or localized increased pressures[17] are all potentially important effects.

For organic transformations involving molecular catalysts, altered reactivity can often be attributed to the absence of solvents, which leads to different energies of transition states and/or intermediates. This can lead to altered reaction pathways, while the proximity of catalyst and reagents in the solid state could enhance rates. Moreover, the fact that mechanocatalysis typically does not require a solvent can be a crucial advantage in reactions of insoluble substrates that can otherwise often not be converted at all. Elucidating the molecular origins of mechanocatalytic effects remains one of the big challenges in this field.

The greatest obstacle in studying the origin of mechanocatalytic effects is the fact that the crucial events in the mill – collisions – are very localized within a few thousands of cubic micrometers, directly affecting only a few micrograms of powder,[18] and occur with short time scales on the order of a few tens of milliseconds,[19] which can be masked by a background of mechanically unagitated material.

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For many years, what happened in ball mills was considered as a 'black box'. This changed when *in situ* X-ray diffraction (XRD) was used to follow the mechanochemical formation of a metal–organic framework (MOF),[20] an approach which was later extended to other techniques and problems, including mechanocatalysis. Despite numerous challenges, the implementation of *in situ* techniques such as powder XRD and Raman spectroscopy for solids has, in recent years, improved our understanding of mechanocatalysis. These approaches allowed intermediates to be identified, the reaction mechanisms and kinetics to be monitored, and relationships between catalyst structures and properties to be established.[21,22]

The integration of other characterization tools during milling, such as X-ray absorption spectroscopy (XAS) or nuclear magnetic resonance (NMR) spectroscopy, further facilitates the understanding of processes occurring during mechanocatalysis at a local, structural level, which will strongly enhance our understanding of the nature of the active centers.[23,24]

Promising approaches relying on the analysis of single collisions, atomic scale experiments, or quantum chemical calculations should provide deeper insights into the crucial factors that control mechanocatalysis, but these have only been pursued to a limited extent.

Single collision experiments have been used in the study of explosives,[25] an AFM-study in combination with quantum-chemical calculations has been used by the Tysoe group to elucidate the influence of pressure,[26] and quantum chemical calculations have been extended from studying mechanochemical reactions in general[27] to mechanocatalysis.[28] If the use of such methods is expanded in the future, we are confident that a deeper understanding of mechanocatalytic reactions can be obtained – and, as it often turns out, that there is often no single cause of the enhanced reactivity, but rather a combination of several effects that are responsible.

Mechanocatalysis has established itself firmly as an important field of mechanochemistry that we are certain will continue to expand. Industrial implementation of mechanocatalysis has not been disclosed, yet this is likely to change in the very near future given its remarkable potential! This will, however, require detailed scale-up studies of mechanocatalytic reactions, essential for mechanochemical processes to be commercialized.

In summary, the area of mechanocatalysis is rich with core questions that remain to be answered, and we hope that this editorial, and the suggested definition of mechanocatalysis, spurs further work and discussion in this area. But whatever the research question or the methodology used, *RSC Mechanochemistry* is the perfect journal for your work, because you will be sure to reach your target audience.

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