ADVANCING SUSTAINABLE SYNTHESIS THROUGH IN SITU MONITORING AND INDUSTRIAL SCALE-UP OF MECHANOCHEMICAL PROCESSES

Franziska EMMERLING,[a,b] Adam A. L. MICHALCHUK[c]

[a] *Bundesanstalt für Materialforschung und -prüfung (BAM), Richard-Willstätter-Strasse 11, and Unter den Eichen 87,12205 Berlin, Germany*
[b] *Department of Chemistry, Humboldt-Universität zu Berlin, Brook-Taylor-Strasse 2, 12489 Berlin, Germany*
[c] *School of Chemistry, University of Birmingham, Edgbaston, Birmingham, B15 2TT United Kingdom*
franziska.emmerling@bam.de

Mechanochemistry has emerged as a powerful approach for sustainable materials synthesis and processing, with significant potential to meet the UN Sustainable Development Goals.[1] This presentation will highlight our recent advancements in understanding, monitoring, and scaling-up mechanochemical transformations, focusing on the balance between fundamental understanding of reaction mechanisms and its practical applications in energy storage and energy transfer materials.
Our research has made significant strides in elucidating the fundamental mechanisms of mechanochemical reactions. We have investigated delayed polymorphism under mechanochemical conditions, revealing new insights into the interplay between mechanical impact, thermal effects, and structural transformations in molecular crystals.[2] By employing variable temperature ball milling, we have demonstrated unprecedented control over polymorphic forms in organic cocrystals, opening new avenues for tailoring material properties.[3]
A central focus of our work has been the development and application of time-resolved *in situ* monitoring techniques for mechanochemical processes.[4] Our research on real-time synchrotron X-ray diffraction has enabled unprecedented insights into reaction pathways and kinetics. Recently, we have successfully applied energy-dispersive X-ray diffraction for time-resolved *in situ* monitoring of reactive extrusion, marking a significant step towards 'lighting up' industrial-scale mechanochemistry.[5]
Bridging fundamental understanding with practical applications, we have explored the mechanochemical synthesis of functional materials for energy storage and transfer, making process in the mechanochemical synthesis of highly proton-conductive metal phosphonates, demonstrating the potential of mechanochemistry to manufacture advanced materials for energy applications.[6] Addressing the challenges of industrial scale-up, we have investigated the role of solvent polarity in mechanochemical reactions, providing valuable guidance for optimizing organic syntheses such as the Knoevenagel condensation.[7] This work contributes to our broader efforts to develop more efficient and sustainable chemical manufacturing processes.
Looking to the future, we will discuss emerging directions in mechanochemistry, including the development of continuous flow processes and the integration of machine learning approaches for reaction prediction and optimization. As we anticipate the next decade of research, we envision mechanochemistry playing an increasingly crucial role in sustainable chemical manufacturing and materials processing, with far-reaching implications for addressing global energy and environmental challenges.

---

[1] J. Alic, M. C. Schlegel, F. Emmerling, T. Stolar, *Angew. Chem. Int. Edit.* **2024**, *63*, e202414745.
[2] K. Linberg, P. Szymoniak, A. Schönhals, F. Emmerling, A. A. L. Michalchuk, *Chem. Eur. J,* **2023**, *29*, e202302150.
[3] K. Linberg, B. Röder, D. Al-Sabbagh, F. Emmerling, A. A. L. Michalchuk, *Faraday Discuss*. **2023**, *241*, 178-193.
[4] A. A. L. Michalchuk, F. Emmerling, *Angew. Chem. Int. Edit.* **2022**, *61*, e202117270.
[5] N. Y. Gugin, K. V. Yusenko, A. King, K. Meyer, D. Al-Sabbagh, J. A. Villajos, F. Emmerling, *Chem.* **2024**, *10*, 3459-3473.
[6] M. Rautenberg, B. Bhattacharya, C. Das, F. Emmerling, *Inorg. Chem.* **2022**, *61*, 10801-10809.
[7] K. Scheurell, I. C. B. Martins, C. Murray, F. Emmerling, *Phys. Chem. Chem. Phys.* **2023**, *25*, 23637-23644.