Mechanochemistry as a green toolbox: from cage molecules to forever chemicals

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Mechanochemistry is a green platform for making materials, triggering solid-state transformations, and destroying persistent pollutants. This talk follows that versatility across two lines of work, both relying on complementary characterisation, including CERIC ssNMR.

First part of talk shows the synthesis and polymorphism of rigid diamond-like cage molecules under thermal and thermo-mechanochemical conditions. Solid-state NMR, obtained through CERIC, confirmed chemical integrity of the material and supported the new crystalline form indicated by diffraction and differential scanning calorimetry. Together with in situ diffraction, these experiments showed that milling lowers the kinetic barrier to a polymorphic transition relative to conventional heating, and that mechanical energy can therefore open a different path to the solid-state landscape.

That same toolbox is now being applied to water remediation of persistent per- and polyfluoroalkyl substances (PFAS). Metal–organic frameworks (MOFs) prepared by milling are used to capture PFAS from water and are then treated again by mechanochemistry to degrade the adsorbed contaminants and recover the adsorbent. The aim is a more circular remediation cycle than incineration or single-use sorbents.

Together, these studies present mechanochemistry as both a discovery tool in molecular materials and a practical method for environmental chemistry, and they illustrate why CERIC techniques—especially ssNMR—are essential for connecting structure, dynamics, and function.

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[c] J. Alić, T. Stolar, Z. Štefanić, K. Užarević, M. Šekutor, *Sustainable Synthesis of Diamondoid Ethers by High-Temperature Ball Milling*, ACS Sustainable Chem. Eng., 11 (2023), 10.1021/acssuschemeng.2c05283
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Short bio:

Jasna Alić Stolar joined the Federal Institute for Materials Research and Testing (BAM) in Berlin, Germany, in September 2024 as an Adolf Martens Postdoctoral Fellow. Since November 2025, she has been an Alexander von Humboldt Postdoctoral Fellow at BAM. She holds a Ph.D. in Chemistry from the University of Zagreb, Croatia. Her research interests include mechanochemistry, with a focus on sustainable organic and materials synthesis, degradation of environmental pollutants and supramolecular chemistry of diamondoid derivatives.