UNDERSTANDING THE MECHANOCHEMICAL REACTION ENVIRONMENT

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Mechanochemical reaction strategies, based on milling, grinding, extrusion and other techniques, have over the past couple of decades demonstrated effectiveness and versatility over a wide range of chemistries and materials synthesis applications.[1] Nevertheless, such mechanochemical reactions generally remain poorly understood, with fundamental, mechanistic, as well as reaction development research focusing largely on the role of mechanical impact and shear. In contrast, considerably less work seems to have focused on characterising the reaction environment under mechanochemical conditions, and the role that such environment might play in enabling or controlling the observed chemical transformations. This presentation aims to address the properties of the reaction environment, effectively addressing the question of *what* is being ground in a mechanochemical reaction, rather than *how* it is being ground. For that purpose, particular attention will be given to experiments that seek to understand mechanochemical reactivity in terms of the reaction environment and the properties of the material being subjected to mechanical processing, rather than in terms of different consequences of impact and shear. Specifically, we will outline our recent work in understanding mechanochemical reactions through new, integrated monitoring approaches that simultaneously investigate the progress of chemical reactions and phase transformations,[2] theoretical modelling of mechanochemical reactions based on molecular dynamics simulations,[3] as well as through exploration of alternative technologies such as Resonant Acoustic Mixing (RAM) as a means to achieve a direct comparison of solution and solventless reactivity.[4]

[1] Friščić, Mottillo, Titi, *Angew. Chem. Int. Ed.* **2020**, *59*, 1018.
[2] Borchers *et al. Chem*, **2025**, 102319.
[3] Ferguson, Friščić, *Phys. Chem. Chem. Phys.* **2024**, *26*, 9940.
[4] Gonnet *et al. Angew. Chem. Int. Ed.* **2022**, *61*, e202115030.