Mechanochemistry: From macroscopic evidence to microscopic mechanisms

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Mechanochemistry is the branch of Chemistry that investigates the effects of non-hydrostatic stresses and plastic strain on the chemical reactivity of molecules, crystals, and other aggregates of matter. Although the directional character of mechanical stresses has been recently shown to enable the selective activation of covalent systems, for centuries mechanochemists focused their work on solids. Dating back to 300 BC, the first written accounts on Mechanochemistry make it one of the most ancient documented forms of Chemistry. Yet, it can be still considered a young science, due to the poor understanding of its fundamental mechanisms. Taking place in the presence of unbalanced mechanical stresses, Mechanochemistry is non-equilibrium Chemistry, and mechanochemical transformations exhibit a typical local character. Mass transport processes different from thermally activated ones occur, which can result in unusual physical and chemical behaviors.The present contribution aims at providing a short overview of the experimental and theoretical attempts performed to deepen the insight into the fundamental mechanisms governing the mechanical activation of solids. Starting from a few representative examples of mechanochemical reactivity, it is shown that accurate kinetic studies coupled with molecular dynamics investigations can throw light on the role of experimental variables and the nature of mechanically activated processes. The potential of Mechanochemistry for the fabrication of new materials, and some of the related challenges, are also briefly discussed.