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Are mechanochemistry and thermal chemistry equal?: probing by nanonewton forces. MARTIN KONOPKA, IVAN STICH, Slovak University of Technology, DOMINIK MARX, Ruhr Universitate Bochum — Chemical reactions can be triggered by different energies, the most common being the thermal energy. Despite the fact that mechanochemistry, where mechanical energy is used instead of the thermal energy was long known, its practical use and impact was limited. Recently advances in experimental techniques, such as atomic force microscopy, fully opened the intriguing possibility to use mechanical energy as a tool for chemical reactions driven by mechanical energy. We use technologically important systems, short-chain (ethyl) thiolated copper clusters and surfaces to investigate the differences between mechano and thermal chemistry. This is an important and opened question as mechanochemistry and thermal chemistry are rarely applied to the same system. Quantum mechanics simulations based on density functional theory indicate that the two chemical reactions are vastly different. While thermal chemistry affects selectively the thiolate-carbon bond, mechanochemistry leaves that bond intact and leads to metal-metal bond breaking processes and creation of unusual high- energy structures nonexistent in the nature.

> Ivan Stich Slovak University of Technology

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