

Title: Understanding of Metal-Organic Frameworks through Mechanochemistry: From Experiment to Theory

Author: Tomislav Friščić

Address: Department of Chemistry, McGill University, 801 Sherbrooke St. W. H3A 0B8

Abstract

Over the past two decades, metal-organic frameworks have emerged as a versatile class of materials for a range of advanced applications, from gas separation and storage to catalysis, leading to recent commercialization.^[1] With our group's interest in the development of new, generally applicable routes to synthesize molecules and materials in the solid state,^[2] this presentation will highlight our efforts in achieving MOF synthesis using ball milling mechanochemistry, i.e. chemical synthesis induced or sustained by mechanical force. The presentation will highlight the benefits of mechanochemistry for MOF synthesis, in terms of reaction speed, efficiency, and the ability to construct complex materials from simple, inexpensive precursors. The use of mechanochemistry for the discovery and understanding of MOF materials will also be discussed, with examples of new phases and framework topologies discovered either by systematic screening of mechanochemical reaction conditions, or by real-time monitoring of mechanochemical MOF formation.^[3] The ability to access new phases, not readily accessible by conventional solution-based routes, also makes mechanochemistry an excellent tool to develop a more thorough understanding of MOF phase diagrams. This will be illustrated by highlighting recent work that combined mechanochemistry and periodic density functional theory (DFT) in order to understand thermodynamic driving forces behind MOF formation, as well as fundamental factors determining the topology and stability of different polymorphs of zeolitic imidazolate frameworks.^[4] Finally, it will be shown how this work opens a door to theoretical prediction and stability evaluation of new MOFs.^[5]

[1] *Nature Chem.* **2016**, *8*, 987.

[2] Do, Friščić *ACS Centr. Sci.* **2017**, *3*, 13.

[3] Katsenis *et al. Nature Commun.* **2015**, *6*:6662.

[4] Akimbekov *et al. J. Am. Chem. Soc.* **2017**, *139*, 7952.

[5] Arhangelskis *et al. Chem. Sci.* **2018**, *9*, 3367.