Mechanochemical preparation of Ruddlesden-Popper type perovskites

N. Biliškov,[1,2] I. Brekalo,[1] V. Martinez,[1] I. Milanović,[3] W. Wegner,[4] T. Pantić,[B.] B. Babić,[3] M. Etter,[5] K. Užarević,[1] T. Friščić[2,6]

[1]Ruđer Bošković Institute, Zagreb, Croatia; [2]McGill University, Montreal, Canada; [3]Vinča Institute for Nuclear Sciences, University of Belgrade, Serbia; [4]University of Warsaw, Poland; [5]DESY, Hamburg, Germany; [6]University of Birmingham, UK

e-mail: nbilis@irb.hr

Understanding mechanistic details of mechanochemical processes enables the optimization of preparational procedures and conditions leading to various important classes of materials. Here, a series of liquid-assisted ball milling reactions leading to Ruddlesden-Popper type perovskites $MCuCl_{4-x}Br_x$ (M = Rb, Cs),[1] monitored *in operando* by synchrotron PXRD will be presented. The results show that the added liquids usually catalyze perovskite formation through a common, unidentified intermediate. However, adding specific strongly interacting liquids leads to stable or metastable solvates, which inhibit or even terminate the perovskite formation. This, in turn, indicates that the role of liquids is not general for all types of systems. Reaction profiles and kinetics, extracted from experimental data supported by computational simulations, will shed more light on the specific role of liquids in inorganic mechanochemical reactions, which has not been widely explored since.

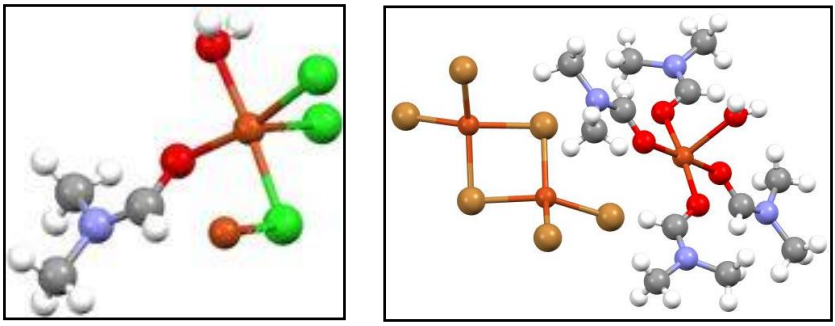

Figure 1 Solvate of $CuCl_2$ and $CuBr_2$ with DMF.

[1] Kundu et al. *J. Phys. Chem. C* **125** (2021) 4720.