

## COST Action CA18112 MechSustInd Training School 2020 Call for trainees

### In situ monitoring of mechanochemical reactions using powder X-ray diffraction and Raman spectroscopy

Date and location: February 23<sup>rd</sup> to February 28<sup>th</sup>, 2020  
Local host: Ruđer Bošković Institute, Zagreb, Croatia  
Address: Bijenička cesta 54, 10000 Zagreb, Croatia

#### About the school

The school will enable participants to understand the advanced topics of *in-situ* monitoring of mechanochemical reactions realized in ball mills. The main topics will cover processing and interpretation of data sets consisting of hundreds of Raman spectra or X-ray diffraction patterns with the intention of extracting reaction profiles for ball-milling reaction. The school will also cover laboratory experimental setup for Raman in situ monitoring, including good practices in data acquisition and data pre-processing. With in situ powder diffraction monitoring being a synchrotron method, trainees will learn how to perform automated Rietveld refinements on previously collected data. The school will cover also the basics of Rietveld refinement using the program Topas.

The school capacity is 10 trainees.

#### Learning outcomes

1. Learn how to prepare the experiment for in situ monitoring of mechanochemical reaction
2. Learn how to setup and align the tabletop Raman spectrometer for data acquisition
3. Learn how to align Raman and powder X-ray diffraction for tandem monitoring and collect data
4. Learn how to apply for beamtime at synchrotron facilities
5. Learn how to process the data, including Rietveld refinement of powder diffraction data

## About MechSustInd

COST action CA18112 Mechanochemistry for Sustainable Industry (MechSustInd) aims at community building of mechanochemists across Europe. Education of young researchers, training of specialised scientists, engineers and technologists, promoting excellence and cross-fertilization among different fields is one of the important objectives of the Action.

## Practical details

The training school lasts 3 full days, starting on Monday 24<sup>th</sup> Feb 2020 and finishing on Wednesday 27<sup>th</sup> Feb 2020. Sunday 23<sup>rd</sup> and Thursday 28<sup>th</sup> are reserved for travelling.

Housing for participants is pre-booked in a nearby dormitory of the School of Medicine of the University of Zagreb at an approximate cost of 30 EUR/day/person.

A grant of up to 700 EUR can be provided for participants as a contribution to the travelling costs, accommodation and subsistence during the Training School.

Trainees are expected to bring their own computers, with ability to install necessary software.

## Application process

Researchers at different ranks are eligible to apply for the training school, including graduate and PhD students, postdoctoral researchers and independent researchers. However, priority will be given to early career investigators (PhD + 8), as well as to trainees from inclusiveness target countries (see [COST ITC](#)), respecting the gender balance.

Applications for the admission to the training school should contain:

- A motivation letter, that provides a clear indication of experience relevant to the topic of the training school; provide a rationale of why you are interested in the training school and how you envisage the training school to contribute to your learning, career and research objectives. (maximum one page)
- A short CV (maximum one page)

Applications for travel grant in addition:

- Estimation of travel costs to and from venue
- Short justification for the travel grant (one paragraph)

Commitment for successful applicants for grant prepare after the training school:

- Follow-up report (maximum one page)
- Feedback for the public website of the action (one paragraph)

Apply by sending email with required documentation to both Martin Krupička ([Martin.Krupicka@vscht.cz](mailto:Martin.Krupicka@vscht.cz)) and Ivan Halasz ([ivan.halasz@irb.hr](mailto:ivan.halasz@irb.hr)), **deadline December 22<sup>nd</sup> 2019**. Please, include **CA18112 TS Application** in the subject field.

## About the host

The Ruđer Bošković Institute, founded in 1950, is public research organisation regarded as Croatia's leading scientific institute in the natural and biomedical sciences as well as marine and environmental research. The institute has a multidisciplinary character: it employs approximately 550 academics and students from the fields of experimental and theoretical physics, chemistry and materials physics, organic and physical chemistry, biochemistry, molecular biology and medicine, environmental and marine research and computer science and electronics.



## School organisers

**Ivan Halasz** has received his PhD in 2008 from the University of Zagreb after which he spent two years as a postdoc at Max-Planck-Institute for Solid State Research. Since 2012 he is a scientist at the Ruđer Bošković Institute working on mechanochemical reactions and in particular their mechanistic understanding. He has been the major developer of powder X-ray diffraction and Raman spectroscopy in situ monitoring techniques.

**Stipe Lukin** obtained his PhD in 2019 from the University of Zagreb under the supervision of Ivan Halasz. In his PhD work, he has developed new methods for data acquisition and processing of in situ Raman data and applied these to various types of mechanochemical reactions. He has co-authored 12 papers including publications in *J. Am. Chem. Soc.*, *Chem. Commun.*, *Chem.–Eur. J.*, and *Cryst. Growth Des.*

## Preliminary programme

Sunday 23<sup>rd</sup> Feb 2020

13:00- Arrival

**Monday 24<sup>th</sup> Feb 2010**

9:30 Meeting at RBI with coffee and cookies

10:00 Introductory lecture (Ivan Halasz/Stipe Lukin)

11:00 Visit to the laboratory at RBI and demonstration of in situ Raman monitoring. (Lukin)

12:30 Lunch

14:00 Setting up synchrotron powder diffraction experiment, introduction to Topas (Halasz)

15:00 Coffee and cookies

15:30 Introduction to Matlab (or Octave) for processing of Raman data (Lukin)

19:00 Dinner

**Tuesday 25<sup>th</sup> Feb 2010**

9:30 Meeting at RBI with coffee and cookies

10:00 Hands-on demonstration of Raman data processing (Lukin)

12:00 Lunch

13:30 Hands-on demonstration of Raman data processing (Lukin)

15:00 Coffee and cookies

15:30 Hands-on demonstration of powder diffraction data processing (Halasz)

19:00 Dinner

**Wednesday 26<sup>th</sup> Feb 2020**

9:30 Meeting at RBI with coffee and cookies

10:00 Hands-on demonstration of Raman data processing (Lukin)

12:00 Lunch

13:30 Hands-on demonstration of Raman data processing (Lukin)

15:00 Coffee and cookies

15:30 Hands-on demonstration of diffraction data processing (Halasz)

19:00 School dinner for all participants

**Thursday 27<sup>th</sup> Feb 2020**

9:30 Farewell and departure

**Martin Krupička**

[Martin.Krupicka@vscht.cz](mailto:Martin.Krupicka@vscht.cz)

CA18112 Training school coordinator