

ONLINE TRAINING SCHOOL WEBCASTED from LISBON March 22-25, 2021

Mechanochemistry: from supramolecular to covalent bonds – synthesis and structural characterization



MechSustInd

ONLINE

Ts@lisbon



OCQE
Química Estrutural

CONTACTS:

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M. Teresa Duarte (Host): teresa.duarte@tecnico.ulisboa.pt

Mechanochemistry: from supramolecular to covalent bonds – synthesis and structural characterization

Date: March 22nd to 25th, 2021

Local host: Centro de Química Estrutural—Instituto Superior Técnico, Lisbon,
Portugal

Address: Online

About the school

The school to be held in Lisbon in March 2021, on "Mechanochemistry: from supramolecular to covalent bonds" will be based on theoretical and pre-recorded "hands-on" experiments in the use of mechanochemistry in the synthesis of supramolecular and covalently bond materials. The expertise of the trainers team embraces both the building of new architectures based on hydrogen and halogen bonds but also the synthesis of new organometallic and catalysts complexes as well as hybrid metal organic frameworks. Different type of mechanochemical approaches will be explained and used, from mortar and pestle to different sort of mills. Classes will also cover some of the characterization techniques available on site: single-crystal and powder X-ray diffraction, ATR-FTIR, Raman, TGA-DSC and ss-NMR, among others.

The school capacity is **30** trainees.

Learning outcomes

The aim of the school is to address some of the diverse synthetic possibilities of mechanochemistry. To show the students the broad applications of the technique, and, at the same time, explain them the theory of the mechanochemical processes. The main goal is to attract new promising researchers to the field of mechanochemistry, showing them the panoply and diverse applications of a solventless green synthetic technique. Introducing the students to some of the most used characterization techniques to study solid materials is an asset as well. We intend to disseminate mechanochemistry as a most important and valuable synthetic technique and show the scientific community its added value. By extending the knowledge on the field, this school will also be a promoter of collaborative networks.

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 4 full days, starting on Monday 22nd March 2021 and finishing on Thursday 25th March 2021.

All sessions will be held online, via zoom sessions.

Trainees are expected to have their own computers, with ability to install necessary software, if required.

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](#)), and 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)

Commitment for successful applicants after the training school:

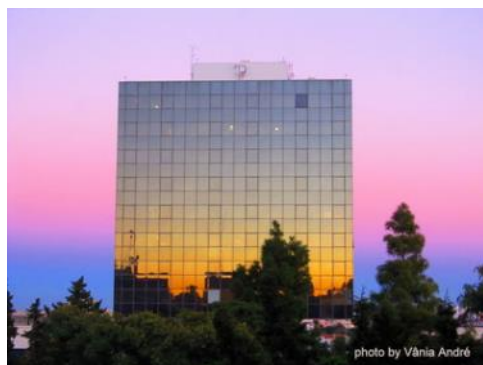
- Follow-up report (maximum one page)
- Feedback for the public website of the action (one paragraph)

Apply by filling the google form available at <http://bit.ly/TSLisbonApp> and send the required documents to Martin Krupička (Martin.Krupicka@vscht.cz) and M. Teresa Duarte (teresa.duarte@tecnico.ulisboa.pt). Please, include **CA18112 TS Application** in the subject field.

Deadline February 21th 2021.

About the host

Centro de Química Estrutural (CQE) is the largest Research Unit of Chemistry of the University of Lisbon (ULisboa), covering a broad and interdisciplinary group of areas within the scope of Chemistry. CQE is a multi- and interdisciplinary unit, promoting also the transdisciplinarity with related sciences, such as materials sciences, biology and medicinal sciences.



It currently gathers ca. 180 Integrated Doctoral Members within a total of ca. 390 registered Members (exhibiting a good gender balance with ca. 54% women) and is organized in 11 research groups which address their research to systems that can have an impact on societal needs, within the following interconnected and flexible 4 thematic lines: Synthesis, Catalysis and Reactivity; Materials, Soft Matter and NanoChemistry; Sustainable Chemistry for the Environment, Energy and Manufacturing; and Medicinal and Biological Chemistry for Health.

School organisers

M. Teresa Duarte has received her PhD in 1989 from Instituto Superior Técnico — Technical University of Lisbon, where she is now Full Professor. Currently she is involved in the design and fabrication of new solid forms of known pharmaceuticals, aiming to stabilize their physicochemical properties and controlling their polymorphism. She has been highly involved with the use and development of mechanochemistry in different synthetic approaches.

Clara B. Gomes obtained her PhD in 2009 from Instituto Superior Técnico — Technical University of Lisbon, after which she worked as a postdoc at CQE (IST-UL). Since 2018, she is the Single Crystal X-ray Crystallography Service responsible scientist and researcher at LAQV-REQUIMTE (NOVA School of Science and Technology). She is interested in the development of new organometallic/coordination complexes, both in solution and by mechanochemistry, for applications in catalysis and for the structural elucidation of target compounds.

Vânia André obtained her PhD in 2011 from Instituto Superior Técnico — Technical University of Lisbon under the supervision of M. Teresa Duarte. She is currently a researcher focused on using mechanochemistry towards new crystal forms (polymorphs, cocrystals, metal-organic frameworks, antibiotic coordination frameworks) of active pharmaceutical ingredients with improved properties and efficiency. She has been acquiring a high level of expertise in Crystallography.

Training school programme (CET time zone)

Monday March 22nd 2021 (10h00 – 18h00)

- 10h00 Opening Ceremony
- 10h30 (T) A mechanochemical process: do we always know what we do not know?
– Elena Boldyreva
- 11h30 Coffee break
- 11h45 (T) X-ray Diffraction: An Introduction – M. Teresa Duarte
- 12h45 Chat room
- 13h00 Lunch
- 14h30 (T) It's not easy being green – a survival guide for the aspiring milling
mechanochemist – Tomislav Friščić
- 15h30 (T) From serendipity to intentional mechanochemistry – Fabrizia Grepioni
- 16h00 Chat room
- 16h15 Coffee break
- 16h30 (Lab) A mechanochemical approach for the synthesis of cocrystals and anti
biotic coordination frameworks – Vânia André
- 17h15 (Lab) Mechanochemistry for life – Vasco Bonifácio

Tuesday March 23rd 2021 (10h00 – 17h45)

- 10h00 (T) Solid-state NMR spectroscopy of small molecules – How it can help with
your research? – Luís Mafra
- 11h00 Coffee break
- 11h15 Flash presentations by students about their work
- 12h45 Chat room
- 13h00 Lunch
- 14h30 (Lab) Efficient mechanochemical catalytic synthesis – Luísa Martins
- 15h15 (Lab) Magnetic materials by mechanochemistry – Ana Ribeiro
- 16h00 Coffee break
- 16h15 (Lab) Solid-State NMR Concepts and Applications – Maria João Ferreira

Wednesday March 24th 2021 (10h00 – 17h45)

- 10h00 (T) IR and Raman spectroscopy: basic concepts – Ermelinda Maçôas
11h00 Coffee break
11h15 (T) Solid State Thermal Characterization – Hermínio Diogo
12h15 (T) Mechanochemistry in action: Exploring different activation parameters
in reactions involving pharmaceuticals – Inês C. B. Martins
12h45 Chat room
13h00 Lunch
14h30 (Lab) Powder X-Ray Diffraction: from Basics concepts to applications
in Mechanochemistry – Auguste Fernandes
16h00 Coffee break
16h15 (Lab) Solid State Thermal Characterization – Hermínio Diogo

Thursday March 25th 2021 (10h00 – 17h30)

- 10h00 (T) Mechanochemistry: from laboratory to large scale synthesis
of Active Pharmaceutical Ingredients – Evelina Colacino
11h00 Coffee break
11h15 (Lab) Single-Crystal X-Ray Diffraction – an overview from basic concepts
to case studies – Clara Gomes
12h30 (T) Mechanochemical cocrystalization: better selectivity and reactivity
– Fátima Piedade
13h00 Lunch
14h30 (Lab) Practical applications of IR and Raman spectroscopies
in multicomponent reactions – Mafalda Sarraguça
16h00 Coffee break
16h15 (Lab) Mechanochemistry with single-screw device – Marta Pineiro
17h00 Closing ceremony (with poll)

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