

CA18112 Mechanochemistry for Sustainable Industry



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***“Mechanochemistry Meets Industry
2nd edition
Economic considerations and
business perspectives***

June 10, 2022



SCAN ME

Book of Abstracts



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Mechanochemistry Meets Industry

2nd edition

**FREE
EVENT**

Economic considerations and business perspectives

June 10th, 2022 – Hybrid event - 12:30 - 16:40 CET

**Aula Magna – Università degli Studi di Cagliari
Dipartimento di Ingegneria Meccanica, Chimica e dei Materiali
via Marengo 2, 09123 Cagliari, Italy**

“Mechanochemistry for Sustainable Industry” - www.mechsustind.eu - **COST Action CA18112**
- strives to advance cooperation between industrial partners and academic researchers to facilitate integration of mechanochemistry into chemical processes at both R&D phase and production scale.

Sabrina CIRILLO (Strategia e Sostenibilità – CIRS srl, Italy)

Roadmap to Sustainability through decarbonization in the industrial perspective

Livia MIAN (CENELEC/CEN, Belgium)

Introduction to standardization system and the role of standards in Research & Innovation

Sabrina SPATARI (Technion, Israel)

Mechanochemical processing can meet environmental and economic sustainability goals

Michael PATRASCU (Technion, Israel)

*Non-smooth modeling paradigm for simulation and optimization of
continuous pharmaceuticals manufacturing processes*

Tanja BENDELE (Ruhr IP, Germany)

*Sustainable Innovations and Intellectual Property IP Strategy for
Sustainable Chemical Manufacturing with Development Support to safeguard the Innovations*

PANEL DISCUSSION – Meet the speakers

SAVE the DATE and JOIN US!

Please register for the live and free event here*: <https://forms.gle/GtTA9uTZ2uV46D119>


Deadlines for registration: May 10th, 2022 – for in person attendance; **June 3rd, 2022** – for online attendance



The detailed program is available in the agenda at www.mechsustind.eu

**MEET THE SPEAKERS, ATTEND
THE PANEL DISCUSSION, AND MORE...**



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* For online attendance, a link to connect will be sent to the registered participants 24 h before the start of the workshop.

Mechanochemistry for Sustainable Industry

The **COST Action CA18112 “Mechanochemistry for Sustainable Industry” (MechSustInd)** focuses on the great promise, and unexpressed potential, shown by Mechanochemistry within the contexts of chemical, pharmaceutical industries, and process engineering.

Organic mechanochemistry has been shown to enable the reduction, or the elimination, of solvents, while ensuring increased yields and scope of substrates compared to solution-phase synthesis, better crystallinity of final products, and access to products that can be formed only under mechanical activation conditions. This COST Action aims at establishing a multi-disciplinary network of European scientists, engineers, technologists, entrepreneurs, industrialists, and investors addressing the exploitation of mechanical activation in the production of chemicals through sustainable and economically convenient practices on the medium and large scales.

Specifically, this Action addresses the objective of harmonizing fundamental and applied research with technological innovation and industrial needs, representing the necessary step for enhancing the impact of mechanical processing onto organic synthesis and transferring specific knowledge into the industrial value chains. The Action aims to nucleate a critical mass of actors from EU research Institutions, enterprises and industries, bringing together different areas of expertise and application. The creation of an authoritative community to promote the study of mechanochemistry and encourage its utilization in production processes will catalyze strategic advances in European chemical industry. The favorable features of mechanically activated (organic) transformations is expected to enable the attainment of far-reaching objectives connected with the development of green economy, the improvement of European market competitors’ capabilities, the innovation of process engineering, and the growth of a new generation of specialized researchers.

Areas of Expertise Relevant for the Action

- Chemical sciences: Green chemistry research
- Chemical sciences: Sustainability
- Chemical engineering: Sustainable engineering
- Chemical sciences: Chemical reactions: mechanisms, dynamics, kinetics and catalytic reactions
- Chemical engineering: Process chemistry and technology



EuChemS

European Chemical Society

EuChemS, the European Chemical Society, aims to nurture a platform for scientific discussion and to provide a single, unbiased European voice on key policy issues in chemistry and related fields.

Representing more than 160,000 chemists from more than 40 Member Societies and other chemistry related organisations, EuChemS relies on a unique network of active researchers involved in all the fields of chemistry. Through this network, EuChemS organises several specialised academic conferences as well as the biannual EuChemS Chemistry Congress, the European congress of chemical sciences. EuChemS also promotes the role and image of the chemical sciences among the general public and policy-makers through social media, newsletters and through the organisation of conferences and workshops open to the society.

Through the promotion of chemistry and by providing expert and scientific advice, EuChemS aims to take part of the solution to today's major societal challenges.

For more information about the European Chemical Society (EuChemS), please visit www.euchems.eu or contact us at:

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“Mechanochemistry Meets Industry” 2nd edition

Economic considerations and Business perspectives

Aula Magna - Università degli Studi di Cagliari, Via Marengo 2

In person, Online and Live Workshop

June 10, 2022

Program

12:30 pm *Welcome cocktail*

Chaired by Evelina COLACINO (Université de Montpellier, France) and Francesco DELOGU (Università di Cagliari, Italy)

13:30-13:50 *Roadmap to Sustainability through decarbonization in the industrial perspective*
Sabrina CIRILLO (Strategia e Sostenibilità – CIRS srl, Italy).

13:50-14:10 *Introduction to standardization system and the role of standards in Research & Innovation - on line & live*
Livia MIAN (GENELEC/CEN, Belgium)

14:10-14:30 *Mechanochemical processing can meet environmental and economic sustainability goals*
Sabrina SPATARI (Technion, Israel)

14:30-14:50 *Coffee Break*

Chaired by Felipe GARCIA (University of Oviedo, Spain)

14:50-15:10 *Nonsmooth modeling paradigm for simulation and optimization of continuous pharmaceuticals manufacturing processes*
Michael PATRASCU (Technion, Israel)

15:10-15:30 *Sustainable Innovations and Intellectual Property IP Strategy for Sustainable Chemical Manufacturing with Development Support to safeguard the Innovations*
Tanja BENDELE (RUHR IP, Patentwälte, Germany)

15:30-16:30 *Panel discussion – Meet the speakers*

16:30-16:40 *Concluding remarks*

LIVIA MIAN



Livia works as Innovation Project Manager at CEN-CENELEC, where she is responsible for different activities aimed at facilitating the integration of the standardization system with the research and innovation community.

INTRODUCTION TO STANDARDIZATION SYSTEM AND THE ROLE OF STANDARDS IN RESEARCH & INNOVATION

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Innovation is paramount in the world of today and tomorrow: the ability to develop new technologies and have them quickly access the market determines who wins or loses in the global economy. In this rapidly changing technological environment, standardization has a fundamental role to play. Standards and standardization are recognized as tools for promoting innovation for both policymakers and businesses, as standards allow to codify knowledge and make it accessible to a wide range of stakeholders.

This intervention will offer an introduction to the European Standardization system and the role of the European Committee for Standardization (CEN) and the European Committee for Electrotechnical Standardization (CENELEC).

The speech will also explain the benefit of integrating standardization with research and innovation activities, showing how standardization creates a foundational framework for innovative and impactful solutions to support the implementation of EU Research and Innovation programmes.

SABRINA CIRILLO



I am an Executive in the ESG field.

I work in Sustainability since 2008, since I became Stakeholder Engagement strategist for a global company in the ICT industry.

I started my career as a consultant in 1998 working in the Business Process Transformation, which I still consider the basis of my approach to change management – and with ESG huge impacts always come along. Now growth paradigms have eventually shifted, now it's much about sustainable growth.

How to achieve this objective is the key value I bring to companies in my professional activity, and this is where my customers ask me to bring them, in order to align them to ESG ratings, to implement UN Sustainable Development Goals and to comply with the Paris Agenda 2030. I support companies in environmental mitigation and adaptation required by EU regulations, as to achieve the Net Zero objective in 2050.

ROADMAP TO SUSTAINABILITY THROUGH DECARBONIZATION IN THE INDUSTRIAL PERSPECTIVE

Sabrina Cirillo, Sustainability Strategist & Founder @ Strategia e Sostenibilità – CIRS srl

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Since Sustainability is always a journey lasting over years and decades, every company needs to fully understand its standing point, before starting and also afterwards.

Main issues to be faced are, on one hand, the objective to reduce carbon footprint and environmental impacts in general terms; on the other hand, the need to comply with a more transparent business model, lower risk and lower-to-none negative social impact.

The way Sustainability works, is by leveraging all the three pillars of the ESG framework: E stands for environment, S stands for Social impacts generated, and G

stands for Governance of the company itself – no achievement is possible without a cultural shift.

What we try to focus on is the possibility to split the overall carbon footprint (CO₂) calculated in accordance with GHG protocol, segregating indirect emissions from the direct ones – the latter being the toughest to be reduced, because they need Innovation and a change in the production paradigm. This quota of CO₂ being, in fact, almost unavoidable (though off-setting is not a chance any longer).

To face this challenge, the solution will come from innovative approaches originated by scientists, spending their lives to create new ways of doing things smarter, with lower impacts, studying new procedures for raw materials and new techniques to reduce, recycle and eliminate waste – like mechanochemistry does.

Industries are now called to action to play their part in the innovation challenge, to struggle against climate change and contribute to Net Zero by 2050.

SABRINA SPATARI



Dr. Sabrina Spatari is an Associate Professor in the Faculty of Civil and Environmental Engineering at the Technion - Israel Institute of Technology. Her research develops and applies life cycle assessment (LCA) methods to support sustainable product development. She has pioneered methods to evaluate the environmental impact of early-stage technology to support the development of green and sustainable chemicals and materials. Dr. Spatari serves as working group 3 leader in CA18112 where she collaborates with Action members on sustainability in scale-up of mechanochemistry processes. Dr. Spatari received her Ph.D. from the University Toronto (Canada). She has authored over 75 peer-reviewed journal papers in industrial ecology.

MECHANOCHEMICAL PROCESSING CAN MEET ENVIRONMENTAL AND ECONOMIC SUSTAINABILITY GOALS

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Mechanochemical methods could play a transformative role in the industrial manufacturing of chemicals and materials. In the pharmaceuticals sector, scaling mechanochemical processes can eliminate use of solvents, reduce excess reactants and make continuous manufacturing of active pharmaceutical ingredients energy efficient if designed holistically with process intensification.¹ The environmental benefits of mechanochemical processes can be evaluated systematically through life cycle assessment (LCA). We present a case example in which LCA was applied to evaluate several sustainability and green chemistry metrics for producing nitrofurantoin, an active pharmaceutical ingredient (API), via continuous twin-screw extrusion (TSE).¹ Compared to conventional solvent-batch synthesis, the mechanochemical process yields significant reductions in energy, climate change and human and ecological health life cycle environmental metrics. Given also major projected cost savings when scaling mechanochemical-TSE, we conclude that mechanochemical synthesis holds much promise for addressing sustainability goals for manufacturing essential APIs and other chemical products.

References

1. Galant, O.; Cerfeda, G.; McCalmont, A.; James, S.L.; Porcheddu, A.; Delogu, F.; Crawford, D.E.; Colacino, E.; Spatari, S. *ACS Sustainable Chem. Eng.* **2022**, *10*, 1430–1439.

MICHAEL PATRASCU



Michael joined the Chemical Engineering Dept. at the Technion in 2020 as Assistant Professor, and established the Process Intensification & Reaction Engineering Lab. His main interests are developing novel intensified chemical processes, using a myriad of computational and experimental techniques.

Before joining the Technion, Michael was a Senior Researcher at ExxonMobil R&D in NJ, USA, and a Postdoctoral associate at MIT, MA, USA.

He holds a PhD in Chemical Engineering from the Technion (2015). Michael is the winner of the EFCE Excellence Award in Process Intensification for the years 2015-2016.

NON-SMOOTH MODELING PARADIGM FOR SIMULATION AND OPTIMIZATION OF CONTINUOUS PHARMACEUTICALS MANUFACTURING PROCESSES

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Process intensification of pharmaceuticals manufacturing by continuous processes is challenged by short campaigns, due to the low volume of most products. This calls for optimization of the entire dynamic campaign to achieve optimal performance. A variety of processes prevailing in the pharmaceutical industry exhibit non-smooth dynamics, rather than discontinuous. A computationally relevant theory of non-smooth DAEs has recently been established, which is suitable for numerical implementations that scale efficiently for large-scale dynamic optimization problems¹. In this talk we advocate a non-smooth differential-algebraic equations (DAEs) modeling paradigm for dynamic simulation and optimization of continuous pharmaceutical process operations. We will illustrate the mathematical modelling of selected processes using non-smooth DAEs, and the resulting non-smooth dynamics². We will demonstrate how the overall campaign performance can be optimized in terms of on-specification productivity and yield. The optimal solutions give very valuable insights on (dynamic) production procedures. We will discuss the implications of using this modeling approach for the analysis and design of novel continuous processes, as well as for technoeconomic analysis.

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TANJA BENDELE



Dr. Tanja Bendele, LL.M. (birth name: Tanja Smolka) is a German Patent Attorney and European Patent Attorney. She studied chemistry with a strong focus on process engineering and reactor technology. During her diploma and PhD thesis in 1995 to 1999 she invented photochromic co-crystals with emerging properties using a mechanochemical process. In 2000, she joined the patent department of ratiopharm GmbH. She also worked in a patent and law firm, with focus on medical technology and set up a consultancy firm for planning experiments for opposition or nullity proceedings in the pharmaceutical sector.

She is counselling European Chemical Industry as well as Industries with software and process-oriented processes. The credo of the law office founded by her is: *We find solutions. Creatively and strategically. With entrepreneurial vision.* She is board member of the German Patent Bar Association (Patent-anwaltskammer) as well as of GRUR Mitte-West and composes professional policy opinions and other publications such as: Sustainable Hydrogen – Climate Protection Objectives and Sector Coupling Accelerate Innovations for Hydrogen Technologies; 09/2021 - CHEManager (<https://www.ruhr-ip.com/en/publications/>). As a member of the board of the German Patent Bar Association she contributes to opinions for the German Ministry of Justice and the EU Commission in regards to intellectual property. Also, she has joined a Master degree course in electrical engineering (E-technology) and information technology, specialising in intelligent energy networks.

Sustainable Innovations and Intellectual Property: IP Strategy for Sustainable Chemical Manufacturing with Development Support to safeguard the Innovations

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Sustainable manufacturing is one of the most common demands of the industry, such as pharmaceutical, chemical, biotechnological industry, is faced with today. In the last century, several mechanochemical methods and apparatus, such as specific ball mills were designed to increase the energy input into the grinding process, to initiate

chemical reactions besides particle size reduction. Many of these innovations were protected by patents and exploited by industry.

A short view into the history of innovations of sustainable manufacturing methods and of apparatuses in patent databases, and an overview of intellectual property rights and their requirements as well as proposals for a mixed synergistic innovation process will be presented.

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