

WORKSHOP RE-INVENTING MATERIALS RESEARCH

*Towards accelerated development by closely orchestrating AI, data,
robotics, and high-performance computing*

**30 JUNE
GRENOBLE**



JUNE 30, 2022 – 8h30-13h30

Maison MINATEC, 3 parvis Louis Néel, Grenoble (or remotely via [ZOOM](#))

Agenda

08:30-08:40 Welcome

08:40-09:40 The digital revolution underway in industrial labs

- *Digitalization in BASF R&D labs - path forward and examples*
Wolfgang GERLINGER, Divisional Digital Officer Group Research, BASF SE
- *The Dow Digital Material Sciences Journey*
Dr. Rui VOGT ALVES DA CRUZ, Senior Regional R&D Director for EMEA, DOW
- *Accelerating the development of Sustainable Materials at Solvay thanks to Digital*
Guillaume Muller, Digital Technology Partner for Growth Platforms, SOLVAY
- *Lab of the Future for battery materials research*
Jeremie Auvergniot, Open Innovation Manager, UMICORE

09:40-10:40 ... and in Research Centers

- *Applications of MAPs and machine learning for the development of solution processed solar cells*
Dr. Jens Hauch, Head of Research Unit High-Throughput Methods in Photovoltaics,
Helmholtz-Institute Erlangen-Nuremberg for Renewable Energies
- *The importance of FAIR data and Data Management Plans in Large Battery Initiatives*
Dr. Ivano E. Castelli, Associate Professor, Head of Studies, MSc Sustainable Energy,
Autonomous Materials Discovery, Energy Conversion and Storage Dpt, Technical University of Denmark
- *Towards Open Semantic Materials Research*
Simon Stier, Head of Digital Transformation, Fraunhofer Institut für Silicatforschung ISC

10:40-11:00 Coffee break

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11:00-12:15 Make it happen! What are the solutions available on the Market?

- *How AI is used by Materials companies today - Characteristics of Success*
Marius-Dan POPA, Director EMEA, CITRINE INFORMATICS
- *Accelerating the process for battery development from electrons to electro vehicles*
Dr Johan M. CARLSSON, Senior Industry Process Scientist, DASSAULT SYSTEMES Deutschland
- *Atinary SDLabs: ML software solutions and self-driving labs to accelerate R&D today*
Loïc ROCH, Co-Founder & CTO, ATINARY TECHNOLOGIES
- *Computational design of materials and processes - machine learning acceleration & multi-level modeling*
Fedor Goumans, Chief Customer Office, SCM Software for Chemistry and Materials
- *Enabling automated labs by next generation material synthesis*
Tobias Coppejans, COO VSPARTICLE NV

12:15-12:50 Focus on policy initiatives

- *Catalyzing Clean Energy Solutions for All*
Mark S Kozdras, Emeritus scientist, Natural Resources Canada
International Co-lead, Mission Innovation's Collaborative Platform: Materials for Energy (M4E)
Canadian Co-PI, German-Canadian Materials Acceleration Centre (GC-MAC)
- **DIADEM - DI**scove**RY** Acceleration for the **D**epl**OY**ment of **E**merging **M**aterials – A French initiative
Mario Maglione, Institut de Chimie de la Matière Condensée de Bordeaux, ICMCB-CNRS, Univ. Bordeaux
Thierry DEUTSCH, Modeling and Exploration of Materials Lab, Univ Grenoble Alpes, CEA Grenoble, IRIG

12:50-13:25 Panel discussion

Prof. Ilian Todorov (EMMC Association) and **Dr. Holger IHSEN** (Helmholtz Association) will join some of the previous speakers to answer the following questions:

- *What are the remaining challenges toward autonomous experimentation?*
- *What are the policies needed to accelerate the deployment of this approach across the Materials Research and Industrial community?*

13:25-13:30 Final remarks and Closure

13:30-14:30 Walking lunch & networking