



The European Materials Modelling Council

<http://emmc.info>

## How the European Materials Modelling Council promotes model development and validation in Europe

*Kersti Hermansson (WP Leader, UU)*

*Pietro Asinari & Luca Bergamasco (POLITO)*

*Adham Hashibon (FRAUNHOFER)*

*Roy Chantrell (UoY)*

*Kurt Stokbro (SYNOPSIS)*

*Volker Eyert & Erich Wimmer (MDS)*

*Nicola Marzari (EPFL)*

*Georg Schmitz (ACCESS)*



**EuroNanoForum  
2019**

**June 12-14, 2019, Bucharest, Romania**

An event of the Romanian Presidency of the Council of the European Union





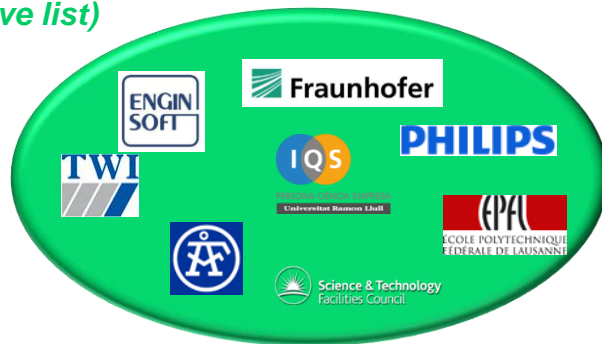
# The European Materials Modelling Council

## The EMMC community

European network (established in Feb. 2014) to coordinate, support and promote the industrial uptake of materials modeling in Europe

### Translators

*(non exhaustive list)*



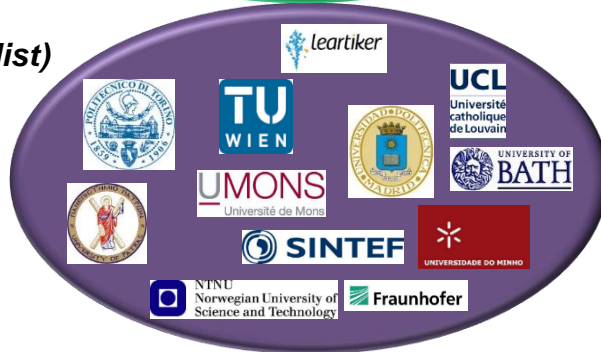
### End-Users

*(non exhaustive list)*



### Model developers

*(non exhaustive list)*



### Software Owners

*(non exhaustive list)*





# The European Materials Modelling Council

## EMMC-CSA: the consortium

### ➤ CONSORTIUM

- ✓ 15 partners from 10 countries
- ✓ 5 companies and 10 RTOs

### Networking

- To strengthen cooperation among different stakeholders throughout Europe (and extra-EU)
- To bridge academic and industrial realities to boost innovation in the materials modelling sector
- To disseminate the results and convince about the potential of materials modelling for industrial innovation





# The European Materials Modelling Council

## EMMC-CSA: The “engine” of the council

### EMMC-CSA

H2020-NMPB project (Coordination & Support Actions)  
to boost the activities of the Council (Sept. 2016)

### WORK PACKAGES

- **WP1: Model Development and Validation**
- WP2: Interoperability and Integration
- WP3: Data repositories and Marketplace
- WP4: Translation and Training for Companies
- WP5: Professional Software Deployment
- WP6: Industrial Integration and Economic Impact
- WP7: Dissemination and stakeholders' community integration
- WP8: Coordination and Project Management
- WP9: Ethics requirements

*"This WP is the key pillar of the CSA activities planned with respect to materials modelling foundations."*



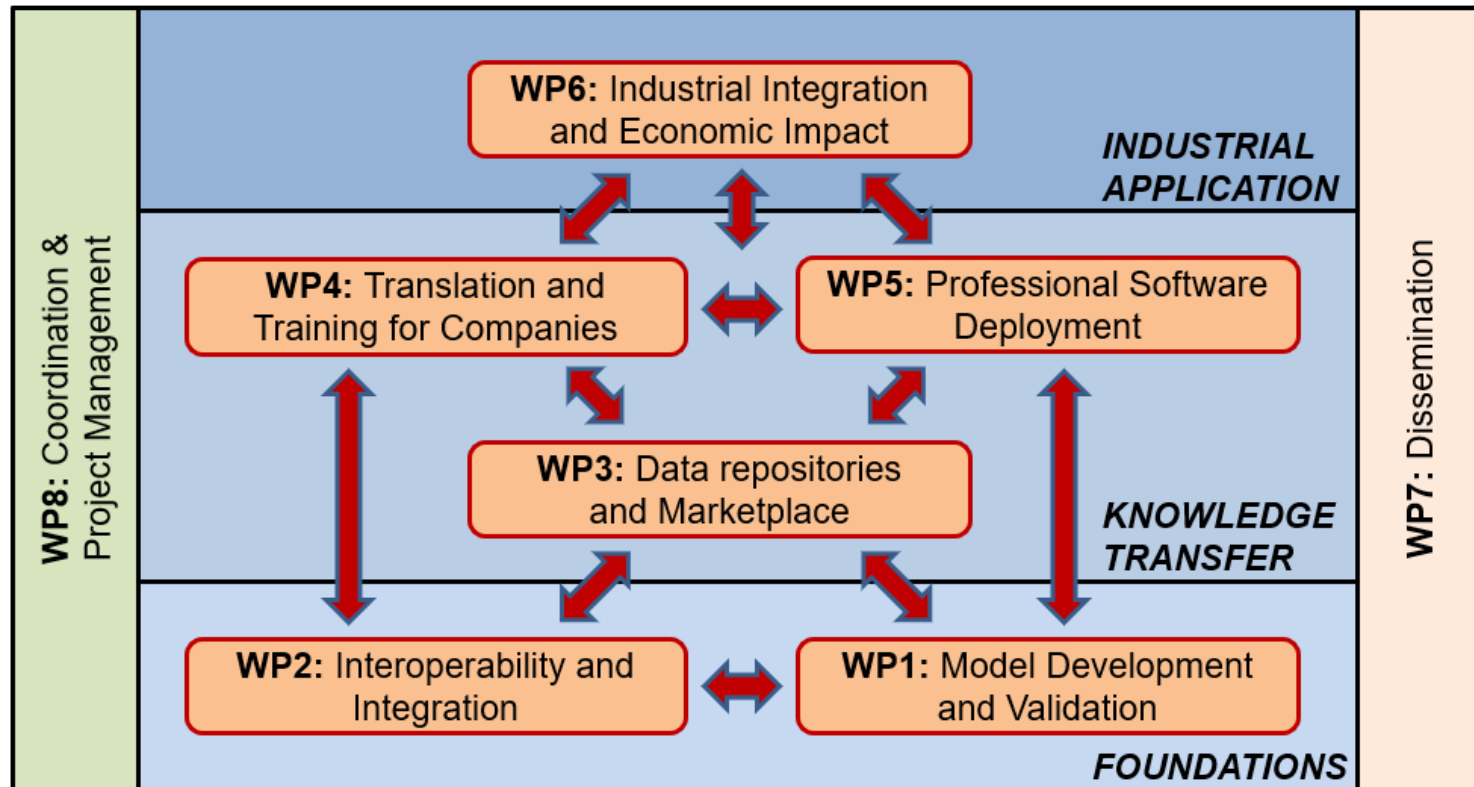


# The European Materials Modelling Council

## EMMC-CSA: The “engine” of the council

### EMMC-CSA

H2020-NMPB project (Coordination & Support Actions)  
to boost the activities of the Council (Sept. 2016)





1. Identify **existing modelling gaps** that need to be filled **by widening models and methods**, prioritise among them, and analyses model development requirements for specific problems relevant to industry to become reachable.
  - Provide guidelines to the scientific community **on how to target scientific efforts towards the needs of the industrial sector.**
  - Special note will be taken of the obstacles connected to **discrete models** as they are severely underused in industry.
2. Define a Roadmap which analyses whether and how some of the existing model gaps can be solved (or mitigated) by **coupling & linking methods.**
3. Define a Roadmap for developing **error estimates for materials models.**
4. Design of a consistent **systematic workflow for validation of materials modelling** with the goal is to strengthen the link between materials modelling and experiments, taking into account existing gaps in the experiments themselves.





## Networking and consultation





# The European Materials Modelling Council

## Networking and consultation

### Other networking activities and consultation

- Networking with CECAM, Psi-k, NOMAD CoE, MaX CoE
- IM2B (our international board)
- Asia Consortium on Computational Materials Science (ACCMS)
- POLITO interacted with NanoHUB at Purdue University

### Recent collaborations

- Pietro A (POLITO) joined the OpenKim management board
- EoCoE (Energy Oriented Centre of Excellence for computing applications)
- Kersti H (UU) in the CECAM Council joint COFUND proposal submitted
- Kersti H (UU) discussions EMMC and Asian Consortium on Computational Materials Science (led from Korea)



<https://www.linkedin.com/company/european-materials-modelling-council/>  
<https://www.youtube.com/c/europeanmaterialsmodellercouncil/>







## Events





# The European Materials Modelling Council

## Model gaps and model development



### 1st EMMC International Meeting

April 5-7, 2017  
Vienna

- The following topics are in focus:
- Model gaps - identification and classification
  - Accuracy and accuracy assessment
  - The roles of software developers
  - Economic impact of modelling
- Remembering that "Gap = Need - Capacity", to remedy these gaps, perform quality assessment, we will thus discuss modelling. The economic impact of modelling (Benefit vs. Cost) needs to be strengthened to promote the use of modelling.

### Boosting the use of modelling

### The 1st EMMC International Meeting

### Meeting organization

### Meeting organization

### Meeting organization

### Meeting organization

### Meeting organization

### Meeting organization



### POLITECNICO DI TORINO

1-2 February 2018  
Sala Giunta, Rettorato  
Politecnico di Torino - Turin, ITALY  
Corso Duca degli Abruzzi, 24

Meeting organization  
Prof. Pietro Asinari - Dr. Luca Bergamasco - Dr. Claudia Sibilla  
Department of Energy - Politecnico di Torino

This event has been financially supported by the EU H2020 project EMMC-CSA H2020-NMPPB-2016-2017 Grant Agreement No. 741874



### Workshops

Coupling and linking simulations - EMMC expert meeting and roadmap  
November 8, 2018 to November 9, 2018  
Location: CECAM-HQ-EPFL, Lausanne, Switzerland  
EPFL on iPhone  
Visa requirements

Registered User Area  
Login: kerz@leem  
Password:.....  
New account  
Lost your password?

- ### Program
- Flagship events
  - Workshops
  - Schools
  - Conferences
  - Node Events
  - Yearly Reports

Details Participants Apply

### Organisers

- Pietro Asinari (Politecnico di Torino, Italy)
- Nicola Marzari (Swiss Federal Institute of Technology, Lausanne, Switzerland)

### Supports



CECAM  
The European Materials Modelling Council

### Description

Algorithms and methods to couple and link multiple model types are often needed to tackle some of the most challenging problems in materials simulations. Developing these represents both a complex and fascinating intellectual challenge, and a pressing need to tackle realistic systems in applied and industrial research.

This expert meeting, convened by the European Materials Modelling Council (<http://www.emmc.info>) and hosted by CECAM, aims to gather some of the foremost experts across different domain areas, with the goal of identifying roadmap for coupling and linking simulations that can act as a manifesto for the field, and inform future policy makers of the algorithmic and methodological developments needed and of their relevance and role in accelerating simulation-driven innovation.

In addition to the invited speakers, self-funded participants will be chosen among the applicants, up to 50 total attendees.





# The European Materials Modelling Council 2019



## Plenary Talk 3

### The nanoporous materials genome in action

by Berend Smit (EPFL, CH)

IMPERIAL BALL ROOM	IMPERIAL BALL ROOM	IMPERIAL BALL ROOM
<b>SESSION 1</b> Bridging physics-based and data-driven modelling  Chair: Kersti Hermansson (UU, SE)	<b>SESSION 4</b> Verification and validation as tools for promoting discrete models in industry  Chair: Roy Chantrell (UoY, UK)	<b>SESSION 7</b> Coupling & Linking of models towards industrial needs  Chair: Pietro Asinari (POLITO, IT)
<b>Impulse presentation #1</b> by Bart Rijkssen (DOW Benelux, NL)  <b>Impulse presentation #2</b> by Signe Riemer-Sørensen (SINTEF Digital, FI)	<b>Impulse presentation #1</b> by David Cebon (Granta Design, UK)  <b>Impulse presentation #2</b> by Jean-François Imbert (SIMconcept Consulting, FR)	<b>Impulse presentation #1</b> by Sabrina Priel (University of Trieste, IT)  <b>Impulse presentation #2</b> by Ludovic Briquet (Johnson Matthey, UK)



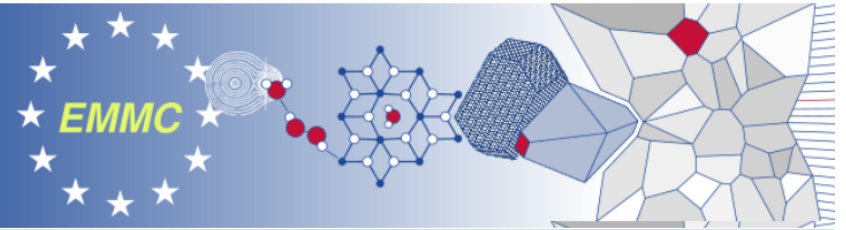


# The European Materials Modelling Council 2019

<https://sites.google.com/site/emultiscale2019/>

Multiscale Modelling of  
Materials and Molecules

2019



Home

Program, venue, and  
Information for  
Presenters

Registration and  
Abstract Submission

Travelling to Uppsala  
and the Ångström  
Laboratory

Hotels

Map of Uppsala

Room location at  
Ångström Laboratory

Organisers

Contacts

## Welcome to the 2019 EMMC-eSSENCE Conference 3-5 June 2019 in Uppsala! (lunch-to-lunch)

*"Multiscale modelling of materials and molecules:  
Physics-based and data-driven."*

**Multiscale modelling** (coupling & linking of models) is a central theme in molecular and materials modelling of complex systems, and it is also a central theme of this meeting. This is the 2nd international EMMC-eSSENCE meeting with the sub-theme of **physics-based & data-driven modelling**.

Future materials and molecular modelling is likely to combine physics-based and data-driven approaches in many new ways. New strategies will emerge to bridge the scales in multiscale modelling, to identify new materials relations and descriptors, and (perhaps) to embark on entirely new S&T fields. Will the reliability, accuracy and validity of modelling improve accordingly? This meeting is about overcoming modelling obstacles in general, with a special focus on solutions that may come from multiscale modelling and from the combination of physics-based & data-driven modelling.







# The European Materials Modelling Council

## 2019: upcoming

<https://emmc.info/events/emmc-torino2019/>

 EMMC Workshop

# Industrial impact of materials modelling

*achievements and perspectives*

July 8-10, 2019 | Turin, Italy





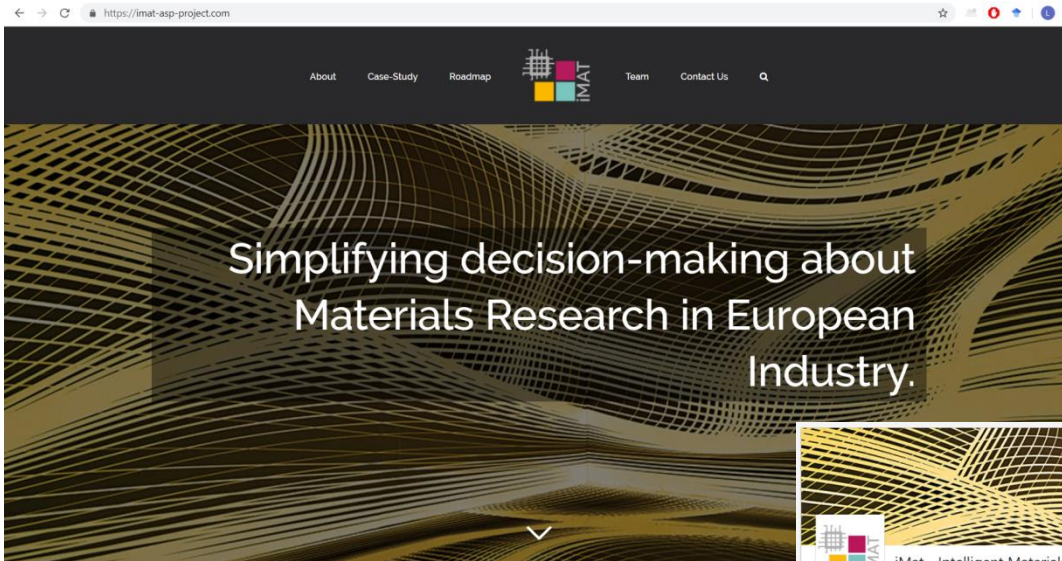
## Education





# The European Materials Modelling Council

## The ASP project: Automatic data extraction from literature



<https://imat-asp-project.com/>

**The results will be available in July 2019 (project ends)!**


### Newsletter

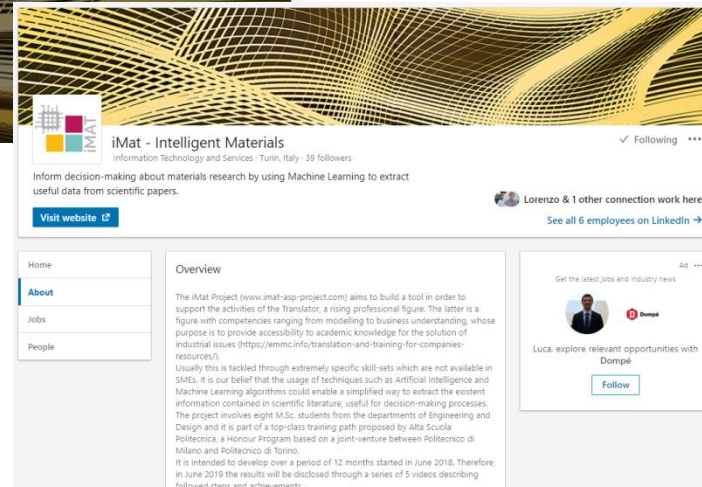
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## Roadmap for novel models







D1.1 Roadmap for the development of novel & improved materials models beyond existing gaps

D1.2 Roadmap for the development of coupling and linking strategies

D1.3 Roadmap for the development of reliable error estimates for materials models (verification) and guidelines to accomplish a systematic workflow for validation of materials models (validation)

**D1.4 White paper on gaps and obstacles in materials modelling → Stay tuned !**





# The European Materials Modelling Council

## White paper

### Guidelines for EMMC-CSA-WP1 White paper on Modelling Gaps and Needs

**Management team:** Kersti Hermansson (coordinator), Pietro Asinari, Volker Eyert, Kurt Stokbro, Roy Chantrell, Georg Schmitz, Luca Bergamasco.



#### Purpose of the White paper

The overriding purpose of the European Materials Modelling Council is to promote modelling in industry. This White paper is a Deliverable for the EMMC-CSA with the label "White paper on gaps and obstacles in materials modelling – and how to overcome them".

However, we also want to publish it as a *real* publication to reach a higher impact. A nice example is the recent open source paper (<https://iopscience.iop.org/article/10.1088/1361-6463/aad926/meta>) by Alberi et al. As you will see, we have borrowed some format features from this publication.

In short, we would like that the document -as a whole- will help to

- 1) promote the use of modelling in industry by highlighting in our texts both today's capabilities and the barriers that need to be overcome,
- 2) inspire scientists to engage in the development of improved models and workflows to overcome the scientific barriers mentioned in our texts,
- 3) promote funding agencies and policy makers, including the European Commission, to promote and invest in actions that support 1) and 2).

*We aim for 2-4 printed pages per author team.*

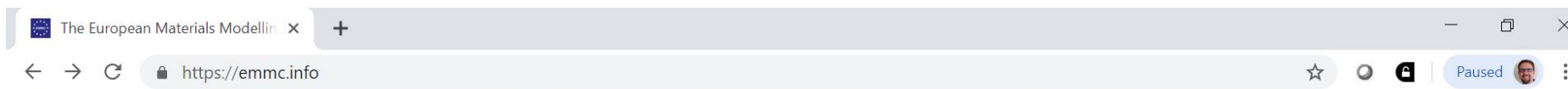
*The text above is taken from the beginning of the writing instructions distributed to the authors of the white paper.*





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Due to ongoing maintenance work, some interruptions of services may be encountered. In this case please retry a few minutes later.

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EMMC-CSA M33 Consortium Meeting  
May 7-8, 2019, Lausanne, CH



