3rd EMMC International Workshop 2021

Proceedings

EMMC ASBL

The European Materials Modelling Council

The European Materials Modelling Council

3rd EMMC International Workshop 2021

March 2-4, 2021

Online

Contents

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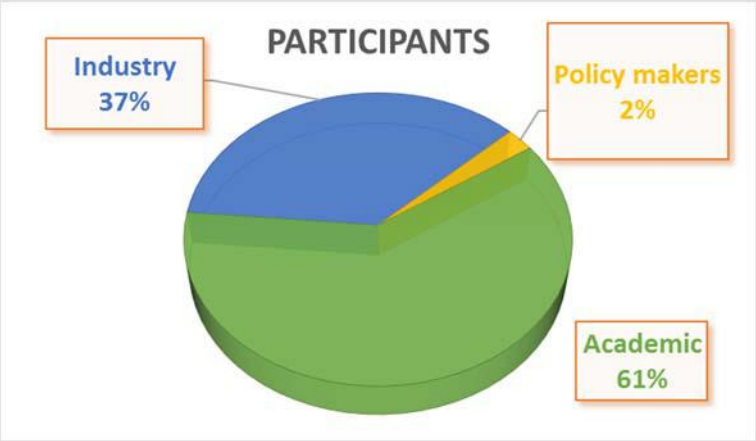
Introduction

The EMMC International Workshop has become known as a leading cross-cutting event where experts from materials, manufacturing and software industries, academia as well as policy and funding stakeholders get together to discuss topics of strategic importance in materials modelling and digitalisation. It is unique in bringing together all types of modelling as well as data science relevant to industrial impact. The format of Discussion Sessions, with prepared Discussion Notes and Impulse Talks by leading experts lends itself to open yet focussed discussion about gaps and potential actions to move the field forward.

Following previous workshops in Vienna in 2017 and 2019, the 3rd EMMC International Workshop (EMMC 2021) took place online from 2nd-4th March 2021.

There were 250 registered participants, mostly from all over Europe as well Israel, Algeria, USA, Canada and Japan. There was again a very significant participation from industry as shown below.



The programme of the event included seven plenary presentations, twelve Discussion Sessions as well as Open Contribution session with online poster and meeting opportunities.

EMMC would like to thank the fantastic community effort in organising and running the event and all speakers and participants for their valuable contributions.

Committees

Organising Committee

Nadja Adamovic	EMMC ASBL President
Gerhard Goldbeck	EMMC ASBL Executive Secretary
Ernst-Dieter Janotka	EMMC ASBL Administration, Events & Communication

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Jesper Friis	SINTEF, Norway
Gerhard Goldbeck	Goldbeck Consulting Ltd., United Kingdom
Adham Hashibon	Materially - The Materials Modelling Marketplace GmbH, Germany
Martin Thomas Horsch	High Performance Computing Center Stuttgart, Germany
Glenn Jones	Johnson Matthey Plc, United Kingdom
Peter Klein	Fraunhofer ITWM, Germany
Franz Pirker	AC2T research GmbH, Austria
Georg J. Schmitz	ACCESS e.V., Germany
Ilian Todorov	UKRI - Science and Technology Facilities Council, United Kingdom
Erich Wimmer	Materials Design S.A.R.L., France

Programme

DAY 1 – Tuesday, March 2, 2021

10:00–10:15 PLENARY ROOM

Nadja Adamovic (EMMC President)
Welcome & The European Materials Modelling Council

Plenary Talks

10:15-10:50 PLENARY ROOM

Plenary 1

Sir C. Richard A. Catlow (University College London and Cardiff University, United Kingdom)

Interatomic Potentials - Why we still need them and how can we improve them

Chair: Kersti Hermansson (Uppsala University, Sweden)

10:50-11:25 PLENARY ROOM

Plenary 2

Emanuele Ghedini (University of Bologna, Italy)

From ontology to practical applications

Chair: Georg J. Schmitz (ACCESS, Germany)

Session 1 TUE, March 2, 2021 11:45-13:15 ROOM ONE

Electronic, Atomistic and Multiscale Modelling: Why should Industry care?

Chair

Maria Alfredsson (University of Kent, UK)

Impulse 1

Ludovic Briquet (Johnson Matthey, UK)
Modelling gaps (and benefits) at the electronic and atomistic levels in industry

Impulse 2

William Curtin (EPFL, CH)
From DFT to precipitation and strengthening in Aluminum Alloys

Impulse 3

Tom Woo (University of Ottawa, CA) - presentation was cancelled!

Accelerated materials design for carbon capture using atomistic and data driven modelling integrated with industrial scale process simulations

Introduction

Numerical simulation in industry today is to a large extent dominated by continuum Structural mechanics and Computational Fluid Dynamics models. They form part of a Computer Aided Engineering design process that started more than 50 years ago and is now regarded as a mature discipline. It is widely adopted in industry and served by a number of multi-billion Euro software companies.

So is there room for, and a need for, materials modelling at the electronic and atomistic levels for industrial problems?

The answer should be yes, as there is a need from industry and society for materials and molecules with tailored electronic, atomistic and nano-scale functionalities. Even the engineering of these materials often relies on controlled electronic and atomic-scale processes. All this is an opportunity for materials modelling, but it is also a challenge to link the microscopic scales to the real world. Capable and reliable models and workflows (physics-based and/or data-driven) will be needed.

The session as a whole is titled Modelling Advances, and the subtheme is the question above: "Is there room for, . . . ?". Our three impulse speakers, and the ensuing discussion, will highlight a range of aspects of how electronic and atomistic modelling can make itself useful, and how weaknesses and scepticisms can be tacked.

Session 2 TUE, March 2, 2021 11:45-13:15 ROOM TWO

Ontologies for Interoperability

Chair

Georg J, Schmitz (ACCESS, DE)

Impulse 1

Colin Batchelor (Royal Society of Chemistry, UK)

Ontologies and Chemistry

Impulse 2

Luca M. Ghiringhelli (NOMAD, Fritz-Haber-Institute, DE)

Ontologies in Computational Materials Science: The NOMAD experience

Impulse 3

Stefano Borgo (ISTC CNR, Laboratory for Applied Ontology, IT)

Applied ontology and its use in product and production modeling

Introduction

An ontology is a formal naming and definition of the types, properties, and interrelationships of the entities that really or fundamentally exist for a particular domain. Recently in the material science domain, various international actions identified ontologies and related information technologies as critical tools for interoperability. Semantic approaches to interoperability arose out of the need to integrate databases having their own data vocabulary, however these have gain attention as ways to facilitate interoperability between heterogeneous materials modelling software in complex workflows.

Session 3 TUE, March 2, 2021 14:15-15:45 ROOM ONE

From Modelling to Experimental Characterisation for Energy Materials

Chair

Malgorzata Celuch (QWED, PL)

Impulse 1

Ferry Kienberger (Keysight Research Labs, AT)

Development of Li-ion battery models from electro-impedance spectroscopy data

Impulse 2

Olivier Douheret (MateriaNova, BE)

Application of modelling tools for the electrical characterisation of organic semiconductors

Impulse 3

Georg Gramse (Johannes Kepler University, AT)

Joint Application of EM FEM and Data-based Modelling for Detection of Small Defect Structures in Batteries

Impulse 4

Marzena Olszewska-Placha (QWED, PL)

Modelling of energy materials and electrical test-fixtures: developments and Open Platform implementation linking MODAs and CHADAs

Introduction

The session aims to correlate computer modelling and experimental characterisation, in application to the increasingly important area of energy materials. Two thematic sub-areas are first addressed: solar cells and batteries, and applications of both physics-based and data-based modelling approaches are considered. Discussion will be directed so as to identify key research problems relevant to the modelling of solar cells, taking into account characterisation data for organic semiconductor materials. Further, industrial problems relevant to the modelling of Li-ion batteries will be discussed, as exemplified by the modelling-based detection of material defects in graphene anodes or separators.

Following the impulse talks, broader discussions and collaborations within the EMMC are envisaged to follow. Expertise in multi-scale multi-physics modelling of energy materials is specifically solicited as well as joint efforts for the development of Open Platform tools and examples, for teaching and public communications on the subject. Collaborations are also sought with the sister society, EMCC, facilitating a MODA of each modelling example to be linked to its corresponding CHADA and characterisation results.

Session 4 TUE, March 2, 2021 14:15-15:45 ROOM TWO

Interoperability in Practice

Chair
Davide Di Stefano (Ansys, UK)

Impulse 1
L. Cate Brinson (Duke University, US)
Working toward Interoperability: Nanomine to Metamine and ontologies

Impulse 2
Gian-Marco Rignanese (Université Catholique de Louvain, BE)
Towards ontologies for databases interoperability

Impulse 3
Jean-Baptiste Lamy (LIMICS, Université Sorbonne Paris Nord, FR)
Tool Suites for Working with Ontologies

Introduction

Material science is evolving from tightly and syntactic connected modelling workflows into more flexible workflows consisting of loosely connected and replaceable modelling software and databases. To exchange data with unambiguous, shared meaning between such loosely couples modelling software that may have been developed independently of each other by groups from different disciplines using different terminology demands an increasingly more explicit and machine-interpretable semantics. Ontologies in the form of logical domain theories and their knowledge bases offer rich representations of machine-interpretable semantics for systems and databases in the loosely coupled world, thus ensuring greater semantic interoperability and integration.

DAY 2 – Wednesday, March 3, 2021

10:00–10:05 PLENARY ROOM

Nadja Adamovic (EMMC President)
Welcome

Plenary Talk

10:05-10:40 PLENARY ROOM

Plenary 3

Nicola Marzari (EPFL, Switzerland)

The digital infrastructures for 21st-century science

Chair: Volker Eyert (Materials Design, France)

Session 5

WED, March 3, 2021 10:50-12:20 ROOM ONE

Digital Marketplaces

Chair

Adham Hashibon, (Materially – The Materials Development Marketplace, DE)

Impulse 1

Martin T. Horsch (HLRS, DE)
Establishing materials modelling marketplaces: from interoperability to cooperation

Impulse 2

Marco Musto (Matmatch, DE)
Material Data Digitalisation Challenges in an Engineering Commercial Environment

Impulse 3

Assaf Anderson (MaterialsZone, IL)
From Design to Manufacturing - the Materials Zone platform

Impulse 4

Amit Bhave (CMCL Innovations, UK)
DOME 4.0 - Enabling interoperability and collaboration in a digital marketplace ecosystem

Introduction

EMMC Digital Marketplaces are multisided collaborative platforms, typically utilising cloud technologies to facilitate the sharing, collaboration, curation, discovery and creation of new insight and knowledge. They typically include integration of several components that can range from translation, digitalisation of research data (covered by a separate session) to education and training and materials modelling applications, requiring thus efficient exchange powered by interoperability between all components. This session is focused on discussing the various interplays between these components, and between various available and emerging public and commercial marketplace platforms.

Session 6 WED, March 3, 2021 10:50-12:20 ROOM TWO

Industrial Requirements to Materials Modelling Software

Chair
Volker Eyert (Materials Design, FR)

Impulse 1
Kurt Stokbro (Stokbro Invest, DK)

Business opportunities for materials science software

Impulse 2
Sophie Loehle (TOTAL, FR)

Speed-up lubricant formulation with computational chemistry tools

Impulse 3
Jonathan Mueller (Volkswagen, DE)

Advancing automotive innovation with materials modelling

Introduction

While materials modelling software is playing an increasingly important role in industrial research the widespread use of these tools is still hampered by a variety of factors. A fundamental issue is posed by the different perspectives of (mostly) academic software developers and industrial end users. Listening to each other and clarifying expectations is thus of key importance for further progress. Addressing the end-user's point of view this session will be concerned with identifying the requirements to materials modelling software. In this context, key aspects include ease of installation, robustness, ease of use, accuracy, complexity, interoperability, performance, training, support, and maintenance. Impulse talks by experts in the field will initiate a discussion about actual and future requirements of industrial end users for materials modelling software.

Plenary Talk

13:30-14:05 PLENARY ROOM

Plenary 4

Bryce Meredig (Citrine Informatics, USA)

Digitalisation of materials innovation

Chair: Gerhard Goldbeck(EMMC Executive Secretary / Goldbeck Consulting, UK)

Session 7

WED, March 3, 2021 14:10-15:40 ROOM ONE

Digitalisation of Research Data

Chair

Martin Thomas Horsch (HLRS, DE)

Impulse 1

Brian Matthews (UKRI STFC Rutherford Appelton Laboratory, UK)

FAIR policies and practices in EOSC

Impulse 2

Jürgen Pleiss (University of Stuttgart, DE)

EnzymeML: FAIR data management in biocatalysis

Impulse 3

Birgit Skrotzki, (BAM Materials Engineering, DE)

Interconnecting data repositories: The Platform Material Digital (BMBF)

Impulse 4

Yann Le Franc (eScience Data Factory, FR)

Building federated FAIR Data Spaces

Introduction

This session addresses ongoing activities and plans concerning

a) the development of research data infrastructures,

b) digitalization of journal data,

providing an opportunity for coordinating between initiatives and planning joint work.

It will be discussed what metadata standards are in use (e.g., MODA, metadata schemas, and ontologies), and how alignment and mediation between infrastructures and journal-publication based knowledge graphs can be supported. The landscape of European-funded projects, including within EOSC, will be evaluated and situated in a global context, in particular as regards the Horizon Europe programme.

Session 8 WED, March 3, 2021 14:10-15:40 ROOM TWO

From Materials Science Software to Industrial Tools

Chair
Ilian Todorov (UKRI - STFC, UK)

Impulse 1
Scott Woodley (UCL, UK)
Development and Evolution of Materials Modelling Software

Impulse 2
Ellad Tadmor (University of Minnesota, US)
Addressing Industrial Needs for Atomistic Simulations through OpenKIM

Impulse 3
Flavio Souza (Siemens Digital Industries Software, US)
Building a Materials Engineering Software Product: From Academic Research to Commercialization

Introduction

This session will focus on the journey from academic materials modelling software to robust tools for industrial use, with examples and tips from experts in the field. Overall, it takes 10 to 15 years to move academic software to marketable software.

To shorten this, innovation and incubation centres at academic institutions can play a major role. Additionally, academic researchers can benefit from introductory business & market training. It is furthermore recommended that academic developments are initiated using a permissive licensing scheme (BSD or Apache), since that's compatible with commercial tool vendors software downstream the innovation chain. Also, the transfer of academic software to industry should be supported more strongly by the scientific community. The continuity of researchers (ending their PhDs, …) is a challenge for long-term academic R&D work.

On the industrial side, software companies should ensure to stay familiar with the state of the art to steer their R&D efforts, avoiding to re-invent the wheel, keeping pace with innovation to match with market needs and focusing on commercialization aspects. Impulse talks by experts in the field will illustrate ways for better transfer of materials science software into industrial tools.

DAY 3 – Thursday, March 4, 2021

09:20–09:30 PLENARY ROOM

Nadja Adamovic (EMMC President)
Welcome

Plenary Talks

09:30-10:05 PLENARY ROOM

Plenary 5

Anne de Baas (Belgium)

Ontology for business opportunities for simulation and comparison of methods

Chair: Denka Hristova-Bogaerd (Dutch Polymer Institute, The Netherlands)

10:05-10:40 PLENARY ROOM

Plenary 6

Søren Bøwadt (European Commission DG Research & Innovation, EC)

Materials modelling and digitalisation - a key enabler for industrial innovation in Horizon Europe

Presented by Javier Sanfélix (DG RTD, EC)

Chair: Nadja Adamovic (EMMC ASBL President / TU Wien, Austria)

10:40-11:15 PLENARY ROOM

Plenary 7

Melanie Herman (Airbus, France)

Challenges for Airbus in the domain of the digitalization of Composite materials

Chair: Patrick de Luca (ESI Group, France)

Session 9

THU, March 4, 2021 11:30-13:00 ROOM ONE

New Developments / Views on Translation and Training for Companies

Chair

Natalia Konchakova (HZG, DE)

Impulse 1

Rudolf Koopmans (Koopmans Consulting, CH)

Scenarios for Industrial Decision Making

Impulse 2

Stijn Donders (Siemens Digital Industries Software, BE)

Ecosystem of a Software Owner towards Translation in Materials Engineering

Impulse 3

Henrik Rusche (WIKKI, DE)

A business model for Translation based on open source software

Impulse 4

Anne de Baas (BE)

Tools for the merge of business economics, translation and decision systems for simulation

Introduction

The Focus Area Impact in Industry has two precursor working groups (WG) of the EMMC, the WG Translation and Training for Companies and the WG Industrial Integration and Economic Impact. While Translation dealt with the transformation of industrial questions to modelling workflows, the Industrial Integration focused on the wide adoption of modelling by the industrial end-users and on the impact of modelling on their business.

One basic idea of the new Focus Area Impact in Industry is to combine these two strands, to build upon the results of the precursors and advice coherent ways for co-creation of innovations by collaborations between industry and modellers, mediated by an advancement of the Translator role.

Session 10

THU, March 4, 2021 11:30-13:00 ROOM TWO

EMMC Roadmap Strategy

Chair

Nadja Adamovic (EMMC ASBL President / TU Wien, AT)

Impulse 1

Erich Wimmer (EMMC ASBL BoD Member / Materials Design, FR)

Implementation strategy of the EMMC Roadmap

Impulse 2

Donna Dykeman (Ansys, UK)

Demonstrating Impact

Impulse 3

Gerhard Goldbeck (EMMC Executive Secretary / Goldbeck Consulting, UK)

Materials Modelling and Digitalisation: a core technology in a post-COVID world

Introduction

The EMMC elaborates roadmaps that identify major obstacles to widening the use of materials modelling in European industry and proposes strategies to overcome them.

The EMMC Roadmap1 is based on input from all stakeholders, including industry end users and materials modelling communities identifying gaps and actions to support the increased utilization of materials modelling in industry. The Roadmap and its implementation address stakeholders from across the value chain, including modelers, materials data scientists, software owners, translators, manufacturers.

Three themes are emphasized in the Roadmap and are linked with R&I projects:

1. Development of Content: providing the *toolbox*
    1.1. Model development and validation
    1.2. Interoperability and integration
2. Development of the Framework for Deployment: making the tools readily accessible
    2.1. Data repositories and marketplaces: Materials Knowledge and Information Management
    2.2. Translation and Training for Companies
    2.3. Industrial Software Deployment
3. Implementation: creating industrial impact
    3.1. Tools
    3.2. Data generation, qualification and validation
    3.3. Processes
    3.4. Workforce Engineering/Talent Development

[1] 2020, The EMMC Roadmap for Materials Modelling and Digitalisation of the Materials Sciences https://zenodo.org/record/4272033#.X7T1WHd2tpw

Session 11 THU, March 4, 2021 14:00-15:30 ROOM ONE

Industrial needs on modelling tools for generating impact in industry and future game changers

Chair
Peter Klein (Fraunhofer ITWM, DE)

Impulse 1
Peter Haynes (Imperial College London, UK)
A View from Academia: the Longest-term Perspective?

Impulse 2
Brian Chol Soo Standen (BASF Corporation, US)
Next Generation computing at BASF

Impulse 3
Thomas Asche (Evonik Operations, DE)
The future, designed by materials modeling - A specialty chemicals perspective

Introduction

Industrial needs on materials modelling are a moving target since the requirements on industrial operations depend on changing regulation, market demands and overall policies (like Green Deal, Digitalization, etc.). On the other hand, completely new computing paradigms, like quantum and neuromorphic computing, show up which potentially will have a huge impact in the long term on industrial innovation processes.

The central question to be answered in this session is: Which features of modelling tools will change the game in industry in the near and long term from the perspective of identified industrial needs?

Session 12 THU, March 4, 2021 14:00-15:30 ROOM TWO

The EMMC Roadmap in the R&I Landscape

Chair
Gerhard Goldbeck (EMMC Executive Secretary / Goldbeck Consulting, UK)

Impulse 1
Esther Hurtós (EURECAT, ES)
Benchmark of R&I programmes with the EMMC roadmap priorities

Impulse 2
Javier Sanfélix & Yanaris Ortega Garcia (DG RTD, EC)
Towards pairing up materials modelling and characterisation

Impulse 3

Erno Vandeweert (DG Defence Industry and Space, EC)
Advanced Materials research and development in the European Defence Fund

Impulse 4

Matteo Mascagni (DG Communications Networks, Content and Technology, EC)
Digital Europe: Path towards Exascale and Quantum Computing. Opportunities for materials modelling and digital transformation

Impulse 5

Alessandro Cavalli (JOINT RESEARCH CENTRE, Directorate C: Energy, Transport & Climate, EC)
Challenges in the Supply Chains for the Green Transition

Introduction

Materials Modelling and Digitalisation is a technology enabler to reach many of the policy goals targeted in the different EU programmes. In this session, funding programmes under preparation for the next multiannual financial framework (MFF) will be identified, where materials modelling and digitalisation has the role to foster innovation in companies.

A benchmark of how these programmes are inter-linked with the EMMC roadmap priorities will be performed, followed by gap identification and proposals for action (e.g. review of work programmes drafts and of EMMC roadmap).

In addition, synergies and coordination needs between the relevant actions in EU programmes will be explored.

3rd EMMC International Workshop 2021

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Online

Talk - Abstracts

MATERIALS MODELLING; ADAPTING THE METHODOLOGY TO THE PROBLEM

Richard Catlow[1,2]

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[2] School of Chemistry, Cardiff University, Main Building, Park Place, Cardiff, CF10 3AT, UK, catlowr@cardiff.ac.uk
https://www.cardiff.ac.uk/people/view/157882-catlow-richard

Key Words: *Interatomic potentials, DFT, QMM/MM, Multiconfigurational system, surfaces*

We review the respective roles of interatomic potential based and quantum mechanical methods in materials modelling and simulation. We identify classes of simulation, where potential based methods are still preferred tool. We then discusses their role in modelling complex multiconfigurational systems, where we focus on the topical case of the surface structure of zinc oxide and show how potential and DFT, methods may be effectively used in conjunction. We describe recent developments in hybrid QM/MM techniques and their application to the electronic structures of the polymorphs of titanium dioxide. Finally, we initiate a discussion as to how potential models may be improved and refined.

From Ontology To Practical Applications

Emanuele Ghedini[1]

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Key Words: *Ontology, Digitalisation, Interoperability, EMMO.*

Everybody who wants to be initiated into the field of ontologies should be ready to embrace a wide range of disciplines that blatantly clashes against the actual tendency towards hyper specialisation of competencies.

Developing effective ontologies to support digitalization of the European industry requires skills spanning through philosophy and logics (for the epistemological approach and ontological formalization), computer sciences (for the tools to exploit ontologies in practice) and the domain experts (such as physicists, engineers, manufacturers), the latter providing the actual knowledge to be ontologised.

This multi-disciplinarity requirement is maybe one of the strongest barrier to be overcome for the effective usage of ontologies, together with the development of tools that will enable the exploitation of the knowledge condensed in ontologies by the largest audience possible.

During the lecture I'll go through the challenge of defining what is an ontology, the ways in which it can be formalized, its potential and limitations, the tools required for its exploitation and some example of usage in practice.

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[2] Morgado, J.F, Ghedini, E, Goldbeck, G, Hashibon, A, Schmitz, G.J, Friis, J, De Baas, A.F. Mechanical testing ontology for digital-twins: A roadmap based on EMMO. International Workshop on Semantic Digital Twins, SeDiT 2020, Heraklion, Greece, June 2020, 2615 (2020)
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DIGITALISATION OF MATERIALS INNOVATION

Bryce Meredig[1]

[1] Citrine Informatics, 2629 Broadway St., Redwood City, CA 94063 USA, bryce@citrine.io

Key Words: *materials informatics, materials design, machine learning, materials data infrastructure*

We discuss the domain-specific characteristics of materials science that make our field simultaneously (1) ripe for digitalisation and (2) a challenging application area for domain-agnostic machine learning (ML). We describe approaches for and benefits of using materials-tailored ML in new materials development; requirements for underlying materials data infrastructure; and unique methodological considerations associated with applying ML to materials data. We conclude by highlighting several emerging areas of materials informatics research.

THE DIGITAL INFRASTRUCTURES FOR 21st-CENTURY SCIENCE

Nicola Marzari

Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), EPFL STI IMX THEOS, Station 9, CH-1015 Lausanne (Switzerland), nicola.marzari@epfl.ch, https://nccr-marvel.ch

Key Words: *Computational Materials Science, Digital Infrastructure, Big Data*

Materials simulations have become powerful and widespread tools for scientific discovery and technological innovation, with billions of euros spent worldwide every year in supporting the researchers deploying these simulations. Applications range from nanotechnology to planetary science, from additive manufacturing to fine chemicals, from semiconducting qubits to Li-ion batteries. Against this backdrop, it is remarkable how comparatively little we plan and invest as a scientific society in developing, supporting, validating and disseminating such a successful research paradigm. The needs and resulting benefits are many, and go from verifying and validating the quantum engines in widespread use, to optimizing their performance on complex architectures, lowering the adoption threshold by enhancing usability and reliability, and integrating data and simulation services. I'll contextualize this with the ongoing worldwide efforts and our own, dedicated to developing and supporting core quantum engines, the AiiDA and AiiDAlab environments needed to provide user-friendly automates simulations [1,2], and the Materials Cloud dissemination platform [3] for curated and raw FAIR data.

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[2] Yakutovich, A.V., Eimre, K., Schütt, M. *et al.* AiiDAlab – an ecosystem for developing, executing, and sharing scientific workflows, Computational Materials Science, **188,** 110165 (2021). https://doi.org/10.1016/j.commatsci.2020.110165

[3] Talirz, L., Kumbhar, S., Passaro, E. *et al.* Materials Cloud, a platform for open computational science. *Sci Data* **7,** 299 (2020). https://doi.org/10.1038/s41597-020-00637-5

ONTOLOGY FOR BUSINESS OPPORTUNITIES FOR SIMULATION AND COMPARISON OF METHODS

Anne de Baas [1]

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Key Words: *Simulation Coaching Technical Translation Decision Systems Ontology*

ABSTRACT

Three strands of the EMMC stand well developed: economics and strategy; technical translation and business decision support systems. First steps are presented to merge and classify these results and to establish relations with the goal to develop ontologies and ontology based tools.

The presented classification of business opportunities for simulation is based on interests that four management levels in a company would have. The interests of each of these management levels are subdivided in at most O(10) subclasses. This first step towards an ontology is also presented in the form of an operational tool, the BOSDA.

This talk will also present a first step towards an ontology for comparison of three information sources (methods): simulation, experiments and reference data. And an operational tool, the COMDA, is outlined.

With the two tools proposes (called BOSDA and COMDA) the gap between the already well developed "technical translation" and "business decisions fed by simulations" will be filled.

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Materials modelling and digitalisation - a key enabler for industrial innovation in Horizon Europe

Søren Bøwadt[1]

[1] European Commission - DG Research and Innovation

Presented by Javier Sanfelix[1]

Key Words: *Horizon Europe, Digital Technologies, Materials Modelling, Sustainable-by-design*

Horizon Europe is the new European Commission Research Framework Programme with a budget of around EUR 95 billion.

It is structured in three pillars, being one of them "Global Challenges and European Industrial competitiveness", where one of the core areas will be on digital technologies and the decarbonisation of the European industry, the so-called Twin Green and Digital transition. These objectives will be addressed within cluster 4 "Digital, Industry and Space". Materials modelling largely contributes to industrial digitalisation, to a data-driven economy and data-sharing practices as it will be presented. Potential synergies to support the green transition will be also covered in the presentation, with a focus on Sustainable-by-Design practices.

CHALLENGES AND OPPORTUNITIES FOR AIRBUS TOWARDS DIGITALIZATION OF COMPOSITE MATERIALS

M. Herman[1], P. Peters[1], S. Cerdan[1], M. Desailloud[1], S. Van der Veen[1]

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ABSTRACT

Application of advanced composite materials to aircraft primary structures is continuously growing, and projects like Airbus A350XWB in the field of commercial aircraft are new references of how far composite technology can be implemented. The validation of those composite parts and qualification of materials is mainly realized by tests. Those tests have an important impact on the cost and the lead time of development project. It is then necessary to develop a numerical alternative to predict the strength and the composite material behavior to decrease the global amount of tests. This numerical alternative would also impulse implementation of innovative technologies with low maturity in future aircrafts development while reducing the time to market. Efficiency for managing evolution of qualified composite materials, competitiveness with multiple sources are as well significant benefits expected from materials digitalization.

To support this target, Airbus is building important bricks to achieve an end-to-end view, with focus on following enablers:

- Simulation of materials behavior, with necessary inputs from material suppliers
- Prediction of materials failure strength by simulation at meso or micro scale
- Simulation of manufacturing flaws and their effect on mechanical strength
- Link between manufacturing process and materials behavior
- Investigation on scale effect: from coupon to structural application
- Management of uncertainties to assess reliability of simulation

Those enablers will be developed to achieve qualification of composite materials with a minimum of physical testing. The presentation will expose the challenges and opportunities for Airbus to develop those bricks towards alleviation of physical testing with an equivalent level of reliability.

Modelling gaps (and benefits) at the electronic and atomistic levels in industry

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Key Words: *DFT, interatomic potentials, battery cathodes, fuel cells, industry*

Being a leading speciality chemical company in the sustainable technologies, Jonson Matthey was an early adopter of atomic scale modelling techniques. The use of computational modelling has grown in the company and DFT and interatomic potential methods are now routinely used in a diverse portfolio of internal projects, ranging from cars' catalytic converters to high energy density Li-ion battery materials. This impulse presentation will focus on our modelling research efforts in the automotive electrification area. I will show how screening several potential dopants using atomistic modelling techniques allowed us to improve the battery performances of our $LiFePO_4$ cathode materials. A selection of dopants is shown to impact charging performance and the cyclability of the cathode materials.
However, despite its successes, some pitfalls remain where DFT methods face difficulty in giving a satisfactory answer. The talk will review the challenges faced in modelling battery materials. Li-ion cathode are particularly difficult to accurately model because they are composed of transition metal oxide with strong electron correlation. In addition, their structure is highly complex with varying oxidation states, dynamic Li migration and the presence of interfaces. One example from our activities in fuel cell development will finally highlight how these pitfalls can manifest themselves when investigating transition metal oxides [1].

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From DFT to precipitation and strengthening in Aluminum Alloys

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Key Words: *Machine Learning, Mechanical properties, Aluminum alloys,*

Industrial processing and application of advanced materials requires exquisite control of both composition and processing path to achieve optimal performance. Bridging the chasm between chemical interactions and macroscopic material behavior can be aided by emerging integrated multiscale materials modelling approaches. Here, we illustrate progress in the domain of metallurgy, presenting a multiscale pathway from first-principles modelling to alloy evolution during processing to alloy yield strength for Al-Mg-Si Al-6xxx alloy. A first-principles database of many metallurgically-relevant structures is created and used to develop a Neural Network interatomic potential (NNP) for the Al-Mg-Si system [1]. The NNP is then used in a Kinetic Monte Carlo study of natural aging to demonstrates that early-stage clusters trap vacancies and delay further evolution at room temperature. The NNP is then further used to compute the Generalized Stacking Fault Energy surfaces for the various β" precipitates formed at peak aging [1], and direct atomistic simulations at experimental scales show the shearing and Orowan looping that control alloy strength [2]. Finally, a mesoscale discrete dislocation dynamics method is calibrated to atomistic NNP quantities and used to simulate Orowan looping in realistic 3d precipitate microstructures [2]. While a seamless multiscale path is not yet complete, our progress to date shows how new machine learning potentials provide a crucial quantitative connection between quantum and meso scales.

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ACCELERATED MATERIALS DESIGN FOR CARBON CAPTURE USING ATOMISTIC AND DATA DRIVEN MODELLING INTEGRATED WITH INDUSTRIAL SCALE PROCESS SIMULATIONS

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Key Words: *multiscale, process simulation, atomistic simulation, data driven*

Metal organic frameworks (MOFs) are crystalline, nanoporous inorganic-organic materials that have attracted significant attention as solid sorbants for various gas separation applications such as large scale CO_2 capture. These materials present an almost infinite design space with innumerable combinations of inorganic and organic building units that can combine to form a permanently porous material. In this presentation, we discuss how data driven modelling has been used to design new materials for post-combustion CO_2 capture that have been realized experimentally and shown to outperform existing materials.[1] We additionally discuss our efforts to integrate atomistic simulations of materials with sophisticated process simulations of the CO_2 capture process[2] with the goal of rationally design materials at the molecular level that are optimized for the industrial process they are to be used in.

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Ontologies and chemistry

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Key Words: *ontology design, name reactions, analytical chemistry*

The Royal Society of Chemistry has developed a number of open-source ontologies for annotating chemical experiments both in organic chemistry, the Name Reaction Ontology (RXNO)[1] and in analytical chemistry, the Chemical Methods Ontology (CHMO).[2] In this talk we describe the methodologies used to develop them, how they have been deployed and how you can take part.

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Ontologies in Computational Materials Science: The NOMAD experience

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Key Words: *Ontology, hierarchical metadata, electronic-structure codes, force-field codes.*

With the tremendous increase in the amount of data in materials science, new ways to store and annotate data are necessary to fulfill the FAIR principles – and to do efficient, good, and new science. Consequently, ontologies have been of increased interest as they do not only allow storing and annotating but also semantically linking data even across domains.

The Novel-Materials Discovery (NOMAD) Repository is the largest database in materials science and provides a normalized, source-independent form of these data in the NOMAD Archive using the NOMAD MetaInfo [1] as metadata schema. The NOMAD Metainfo includes a number of relations between concepts and therefore already goes beyond the simple metadata concept. We have converted it to an ontology and extended it to increase semantics based on the European Materials and Modeling Ontology (EMMO).

Furthermore, within the NOMAD ecosystem, we have created an ontology collection covering materials structures and properties in a more general semantic way. We demonstrate how this may enable connecting multiple sources of knowledge and allow for semantic searches.

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Applied ontology and its use in product and production modeling

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Key Words: *Ontological analysis, Ontology, Product, Process, Functionality, Resource*

Applied ontology (AO) has been introduced to overcome interoperability problems across information systems and today is used in domains as different as finance, medicine, geography, engineering and digital heritage. AO is intrinsically multidisciplinary and deserves to be introduced twice: we first introduce AO as a way of thinking and then as a tool for modeling. The second part of the talk is about the use of ontology in industrial activities. These activities are rich data producers and usually a company exploits several information systems targeting different tasks and users. The talk presents some (good and not so good) applications of ontology in manufacturing and discusses challenges like the modeling of product functionality and of resources in production planning.

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Development of Li-ion Battery Models from Electrochemical Impedance Spectroscopy Data

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Key Words: *battery modelling, battery characterization, electrochemistry, modeling*

The reliable electrical testing and diagnostic evaluation of battery cells, modules, and packs is currently an important task in industrial automotive manufacturing and in battery field tests. Here we present how calibrated and accurate experimental data acquisition is combined with electrochemical modeling for robust data interpretation. The combined electrochemical impedance spectroscopy (EIS) measurement hardware, calibration procedure, and modeling software allows for the analysis of different cell form factors and power levels. We show how EIS output data is used as input data to modeling algorithms to extract the equivalent electrical circuit parameters of the cell. The resulting model is amenable to electro-chemical interpretation and provides a compact representation of the detailed performance characteristics of the cell, relevant for evaluating the SoH (State of Health) and second life applications of cells, modules, and packs. A standard operating procedure (SOP) is provided for EIS focusing on metrological evaluation of accuracy and error sources for low impedance battery measurements. This is developed in ongoing EU research projects (e.g. NanoBat) and evaluated in round-robin tests together with OEMs and national metrology institutes. Accurate experimental workflows, metrological measurements, and modeling are brought together for robust industrial use cases, for instance in battery manufacturing Gigafactories.

Application of Modelling Tools for the Electrical Characterisation of Organic Semiconductors

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Key Words: *Organic semiconductors, charge transport, space charge limited current, Maxwell coupled drift and diffusion, Analytical modelling.*

With the discovery of (semi)conducting properties in organic materials, organic electronics have progressively emerged as a complementary technology to microelectronics. Organic semiconductors now compose several key electronic devices to be considered for IoT applications, with added value such as large scale and low production cost, mechanical flexibility, and low environmental footprint. While industrial developments are taking longer time to happen due to crucial challenges still to be overcome, academic research has been exhibiting an ongoing enthusiasm in the field, sustained by the huge diversity of materials to be studied [1]. Especially, unravelling the conductive properties in these materials remains an open and complex challenge ought to the different mechanisms likely to impact the charge transport, even further leveraged by the diversity of materials. The current solid and powerful modelling tools offered by quantum chemistry is driving the molecular design and synthesis for ultimate performance at atomistic and molecular scales [2]. At mesoscopic scale and beyond, different (semi-)empirical models independently shaped out with time from experimental protocols and associated physical formalisms. This results into large disparities in the estimation of key semiconducting properties of the materials, typically the carrier mobility, thus questioning the pertinence of the existing models and striking the need of consistency in modelling endeavours likely to serve the disentanglement of the different mechanisms contributing to charge transport in bulk materials.

This work proposes to illustrate such challenge for the modelling of bulk carrier transport in a reference semiconducting polymer (poly-3-hexylthiophene, P3HT [1]) coordinating different experimental protocols with their different probing scales and mechanisms. The amorphous or bare polycrystalline organization of organic semiconducting thin films fosters dominating charge hopping among transport mechanisms. The resulting carrier mobilities are sufficiently low to make the material exhibiting space charge limited current (SCLC) regime upon low electric field [3]. Associated models are analytically derived considering drift and diffusion equations and the geometry of the device under test. Their suitability for the determination of carrier mobility is demonstrated for a macroscopic and planar hole-only device geometry and a nanoscale hemispherical tip-sample contact configuration [4]. SCLC is evidenced and consistent carrier mobility is determined evidencing similar leading transport mechanisms in bulk P3HT down to the mesoscale. The derived values are shown to describe interchain transport in the orthogonal π-stacking of the polymer backbone [5]. Exploring intrachain transport can be carried out using microwave characterisation methods [1], which typical operating frequencies correspond to temporal response of polaronic transport. Dielectric resonators and scanning microwave microscopy recently demonstrated sensitivity to variations

of electrical properties in polythiophene, at the macro- and nanoscale, respectively [6,7]. In dielectric resonator, standard Maxwell model is augmented data filtering to derive the complex permittivity of the material and prepared to be coupled to drift-diffusion in further work. In SMM, a home-made analytical model considering the interferometer-based detection unit is currently under validation to also derive locally the complex permittivity. Comparing intrachain and interchain bulk electrical properties shall then serve for material screening to determine their ultimate bulk performances and evaluate the fabrication and integration in electronic devices.

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Joint Application of EM FEM and Data-based Modelling for Detection of Small Defect Structures in Batteries

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Key Words: *Multiphysics finite element modelling, Battery characterization, combined measurements and modelling.*

Lithium-ion batteries (LIBs) are currently the most relevant energy storage solution for a wide field of applications starting from mobile communication and going to high power applications in electric vehicles. Reliable production of the batteries requires measurement techniques and electrochemical models capable to assess possible failures in the production process. Here we will discuss two approaches for LIB quality inspection based on the measurements of the DC self-discharge current and the electrochemical impedance spectroscopy combined - both compared to the respective modelling.

To assess the quality of a LIB either during production or in post-production, its self- discharge rate is an important parameter. Here we present both precise potentiostatic self-discharge measurements (SDMs) on commercial LIBs, and modelling of the SDM which includes the electrochemical processes that are coupled with a 3D temperature FEM and an electric circuit model of the cell self-discharge [1]. Our modelling results in a good overlap with the experimental results and allows us to extract a quantitative value of the LIB self-discharge resistance. Furthermore, we tested a realistic physical self-discharge scenario of the formation of Lithium dendrites by comparing experimental and modelled self-discharge resistance values. Finally, a short overview of our current work on Electrochemical Impedance Spectroscopy (EIS) for following battery's aging processes will be presented [2]. EIS is a potentialnon-destructive method for characterizing and modelling the dynamic behaviour of electrochemical systems such as batteries. We combine this technique with microscopic and nanoscopic measurements to establish and validate our electrical finite element models of the complex and highly parametrized model of a LIB.

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Modelling of energy materials and electrical test-fixtures: developments and Open Platform implementation

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Key Words: *Energy materials, batteries, organic semiconductors, Maxwell equations, heat transfer, drift-diffusion equations, multiphysics modelling, coupling and linking, GUI.*

This talk addresses three aspects pertinent to the progress in materials modelling: model developments, their validation against laboratory experiments, and last but not least, dissemination and popularisation via EMMC activities and open research platforms.

The EMMC assembles groups active in the developments of different material model types and even more such models are available on the European research area. Typically, each model comes with its own user interface, and in many cases the model cannot be practically used by anyone except its authors. This is especially true in the case of emerging technologies and new materials, such as energy materials, where the scientific progress in the models is much faster than computer interface developments may reasonably follow. This hinders the models' validation, interoperability, and general use. Herein, we consider a solution alleviating some of those obstacles, while seeking a compromise between the open innovation and the commercial interest of the European software companies.

- In the first part of this talk, we discuss our physics-based modelling approach, which originates from the electromagnetic modelling algorithms, subsequently coupled to thermal solvers and amalgamated in QuickWave software [1], for which industrial impacts have previously been shown [2].
- In the second part, we present how our modelling helps design material test-fixtures and experiments for energy materials' testing at GHz frequencies. We illustrate this part with selected results of dielectric resonator measurements organic semiconductors and graphene anodes.
- In the third part, we present our Open Platform initiated in H2020 MMAMA [3][4] and currently developed in the NanoBat project [5]. The Platform is based on a common, interoperable, licence-free GUI and a built-in expandable library of User Cases. The GUI invokes licence-free solvers relevant to teaching and basic research as well as commercial solvers appropriate for larger-scale industrial applications.

With this talk, we seek collaborations on extending the Open Platform with new multiscale models and linking-coupling procedures, for which purpose a Task Group is being proposed with the EMMC Focus Areas #1 and #2.

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Working toward Interoperability: Nanomine to Metamine and Ontologies

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Key Words: *Materials properties, Polymers, Ontology, Knowledge Graph*

Data-driven methods can help accelerate materials design given the vast array of past research data. Data resources that hold these research data in a findable, accessible, integratable, and reusable (FAIR) way are essential to the success. NanoMine is an ontology-based, open-source data resource that follows the FAIR principles for the polymer nanocomposite community. During the development of NanoMine, a standalone API service entitled ChemProps was developed to solve the database indexing issue caused by the lack of uniformity in polymer names, which integrates seamlessly into NanoMine platform and enables more interoperability across many polymer data sites.

Beyond being a contribution only to the polymer nanocomposite community with the NanoMine Knowledge Graph, NanoMine has the vision to create the Materials Knowledge Graph as a stable, user-friendly data and knowledge framework for materials through the development of an extensible semantic infrastructure with customized and customizable user templates and semi-automatic curation tools for data entry and associated data validation protocols, along with ontology-enabled design tools and custom user dashboards.

The first sibling of the NanoMine Knowledge Graph under the Materials Knowledge Graph framework is the MetaMine Knowledge Graph, which extends from the NanoMine schema and ontology, which by itself is also an extension of the work done in modeling entirely different domains, including epidemiology and bioinformatics. By building off an existing science ontology (Semantic-science Integrated Ontology, or SIO), the extension into a related metamaterials domain is smooth, since most of the modeling was done and only a few tasks including how to describe metamaterials geometries, and how to represent modulus tensors are left to be considered.

TOWARDS ONTOLOGIES FOR DATABASES INTEROPERABILITY

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Key Words: *Materials Databases, Application Programming Interface, Ontologies.*

In the last decades, a number of materials databases have become available online (see e.g. Ref. [1] for an extensive, yet inevitably incomplete, list). In many cases, these can be accessed via a graphical web interface which targets a "low-throughput" human usage but that is not very well suited for a systematic "high-throughput" computational approach. In fact, in order to take full advantage of modern data-analytics techniques, it is essential that these databases also become accessible through an application programming interface (API) as it is already the case for some of them [2-5]. It would actually be even more beneficial to have access to information originating from multiple databases as they often cover different material families and properties. Nonetheless, retrieving data from multiple databases is difficult since the available APIs are different from one database to another.

In order to overcome these problems, the OPTIMADE API was developed. It was designed so that it can be implemented without significant changes to the established back-end code, and, furthermore, adopting the API is straightforward for the end user. The OPTIMADE specification version 1.0.0 was released on 1 July 2020 [6]. It is supported by leading databases such as AFLOW, the Materials Cloud, the Materials Project, NOMAD, OQMD, ... Currently, the returned properties comprise both mandatory information about the structure (such as the elements the lattice vectors), as well as optional and database-specific information prefixed with the database name (e.g., _aflow_).

In this talk, I will outline some key features of the API specification. I will illustrate its usage through some examples. Finally, I will discuss how it would benefit from more fundamental work on an ontology for materials databases.

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Tool Suites for Working with Ontologies

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Key Words: *Ontology Tools, Ontology, Python*

Ontologies are currently the most expressive model for formalizing complex knowledge. However, after modeling an ontology, one often need to connect it to other component, such as a dynamic website or a database. Since more that seven years, the Owlready Python module is developed for facilitating the use of ontology in Python. This module offers the best of three worlds: (a) formal ontologies, with automatic reasoning capabilities, (b) relational databases, with fast access time and huge volume support, and (c) agile programming in Python, with the ability to quickly write scripts and applications.

A data-model driven approach for semantic interoperability in scientific software

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Key Words: *Data modelling, interoperability, technology adoption, scientific software.*

ABSTRACT

The European Material Modelling Ontology (EMMO[1]) formalises knowledge representation of materials, modelling and characterization. The emerging technology for enabling semantic interoperability, has not been widely adopted in the industry yet. Feedback from data- and application providers indicate that industrial onboarding is a challenge. In industrial applications, the structure and knowledge about existing data is often well known., and metadata and/or data schemas can be provided with little effort. However, the ability to map this knowledge to an ontology and/or develop a new domain ontology requires special expertise. To construct domain ontologies and/or map information to ontological concepts (i.e., EMMO concepts) requires training on semantic technologies and an understanding of the fundamental idea behind the structuring of the ontology. Here we present a data model that represents the physical perspective i.e., provides a data-representation close to the physical data source. The data model can be included in a representation of the logical perspective i.e., the relationships between multiple data models in a software system. Furthermore, the data model can be enhanced further by mapping its properties and attributes to ontological concepts that describes the information from a conceptual perspective. Importantly, the mapping can be performed in retrospect, by someone other than the original provider of the data model. Furthermore, the syntactical data model representation can be tailored to fit the most technical needs, with formats such as JSON, YAML, XML etc. The data model can also be realized as RDF-triples that maps to concepts in representational frameworks such as EMMO, supporting semantic representation (mapping). The RDF-triple representation allows for the later adoption of the mapping.
We show that it is possible to accelerate the onboarding process by defining knowledge-base- and database agnostic data-models that can be retrospectively mapped to ontological concepts and specific data points.

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ESTABLISHING MATERIALS MODELLING MARKETPLACES: FROM INTEROPERABILITY TO COOPERATION

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Key Words: *semantic interoperability, marketplaces and digital platforms, FAIR* .

Designing a system of interoperable marketplaces has been central to the European Commission's strategy for digitalization in materials modelling within the LEIT NMBP line of the Horizon 2020 research and innovation programme. This includes the Virtual Materials Marketplace (VIMMP), MarketPlace, MARKET4.0, and DOME 4.0. This impulse talk summarizes work in progress concerning semantic interoperability from the point of view of the VIMMP project, with a focus on perspectives for interoperating with other marketplaces and digital platforms. Challenges are identified regarding the uptake of the FAIR principles in domains of knowledge from materials modelling, aiming at discussing the best way forward jointly with the participants of the EMMC International Workshop.

This impulse presentation is given on behalf of UKRI Science and Technology Facilities Council (STFC). The Virtual Materials Marketplace (VIMMP) project is funded from the European Union's Horizon 2020 research and innovation programme under grant agreement no. 760907.

MATERIAL DATA DIGITALISATION CHALLENGES IN AN ENGINEERING COMMERCIAL ENVIRONMENT

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Key Words: *Data Digitalisation, Applications*

There are significant benefits to be reaped from large material properties datasets sharing a common, efficient format. One emerging application enabled by material data digitalisation is the ability for the custom design of materials via property prediction [1].
On the other hand, applications relevant to the practising engineer such as for example material selection or structure optimisation have yet to leverage the advantages of digitalised material data. This talk will attempt to clarify some underlying challenges.
Firstly, as the material needs to be described at longer length scales, say from grain to subcomponent scale, the level of complexity explodes. The data volume alone, required to describe in detail for example the processing history, grows very rapidly. While this aspect can be handled by the use of efficient data structures [2] and cloud computational tools, difficulties are exacerbated by the lack of agreed definitions and truly standardised test methods. As an example, the number of "hidden variables" present in a universally accepted test methods will be highlighted. Furthermore, there are commercial obstacles preventing efforts towards a truly standardised description, which the authors encounter during their daily activities.

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From Design to Manufacturing - the Materials Zone platform

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Key Words: *Collaborative platform, AI/ML, Interoperability, Materials, Manufacturing*

Materials Zone is a scientific AI/ML-based collaborative platform.

By harnessing data, technological tools, and years' worth of extensive know-how and experience, Materials Zone accelerates R&D and Manufacturing processes and reduces costs across industries. The MZ platform funnels both R&D and Manufacturing data into an interoperable and structured data-base and enables to manage work processes efficiently, collaborate, achieve meaningful AI/ML insights, and drive better decision-making.

www.materials.zone

DOME 4.0 - Enabling interoperability and collaboration in a digital marketplace ecosystem

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Key Words: *Open Innovation, Marketplace, Interoperability, Advanced Materials, Manufacturing, Data Space*

The Digital Open Marketplace Ecosystem (DOME) 4.0 aims at providing a comprehensive industrial open data ecosystem aligned with the Open Science and Open Innovation objectives for the purpose of value generation and creation of new or enhanced products, processes and services. Given the significant contribution of the materials and manufacturing sectors to the European economy, DOME 4.0 focuses on data-driven knowledge generation within these key sectors.

The DOME 4.0 project, in its first quarter sets the vision for enabling semantic interoperability and connections with existing marketplaces, open simulation platforms, open translation environments, etc. in advanced materials and manufacturing domains. The execution of this vision entails nine B2B showcases comprising interoperability across heterogeneous data and software, as well as cross-domain decision making.

The focus of this impulse presentation is to foster discussion on the challenges and the solutions space in developing a marketplace ecosystem based on FAIR data principles.

Business opportunities for materials science software

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Key Words: *Atomic-scale modelling, electronic-structure methods, Quantum Computing, Market Analysis, Business startup.*

In 2002 my research group developed a new methodology for simulating electron transport in nanoscale systems[1] which today has become the de-facto standard for ab'initio modelling of electron transport. Instead of making the methodology freely available in an open source software package I decided to pursue a non-conventional avenue in the European electronic structure community and make it a commercial software product, what today is the QuantumATK package[2]. QuantumATK is today part of Synopsys and used by all the major semiconductor companies for developing next generation technology nodes and 35 full time employees are involved in the development, support and sales of the package. I will analyze how we could successfully enter the very competitive market for commercial atomic-scale modelling software and discuss some of the opportunities that exist today for new entrants.

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Speed-up lubricant formulation with computational chemistry tools

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Presented by A. Mavrmaras, Materials Design, France

Key Words: *Molecular modelling, additives design, lubricant formulation, Computational Chemistry*

ABSTRACT

Lubrication plays a major role in a wide range of key sectors such as automotive and industry. Renewal of lubricants is currently triggered by the quest of improved properties together with reduced environmental footprint. Molecular modeling is a powerful tool that already proven its ability in understanding reactivity of lubricant additives toward a surface [1-5] and combined with machine learning method, can screen candidates within defined physical-chemical properties [6]. An example will be presented in order to show how a fundamental study can be applied to an industrial issue and what will be the future challenge in computational chemistry.

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ADVANCING AUTOMOTIVE INNOVATION WITH MATERIALS MODELING

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Key Words: *Materials Modelling, Materials Design, Industrial Research & Development.*

Materials modelling software holds great promise for industrial research and development efforts in the face of diverse materials challenges. Bringing a new materials-based product to the market requires various stages of materials research and engineering. Materials modelling software should be designed to address the unique challenges faced at each stage of a product's development. Approaches to overcoming these challenges are not to be primarily evaluated based on their formal correctness, but on their ability to successfully advance the development of new technologies made possible by novel materials.

FAIR Policies and Practices in EOSC

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Key Words: *FAIR, policies, principles, data, EOSC, tools, practices*

Abstract

The FAIR principles (Wilkinson et al., 2016) offer guidelines on delivering research data that is accessible and reusable, while allowing the rights of researchers to be respected. They have become a central concept in the development of research infrastructure, and in particular the European Open Science Cloud, an effort to federate research e-infrastructures across Europe and beyond into a common data ecosystem. The EOSC has coordinated the development of policy and practices to encourage the publication and use of FAIR data. However, how these principles can be realised in practice for researchers working in particular research areas remains a subject of further exploration.

In this presentation, we shall discuss these aims and approach of the EOSC in advocating FAIR data. We shall further consider how these aims might be reflected in the research practice of scientists working in physical sciences. In particular, we shall present the work of the ExPaNDS project in enabling FAIR data from experimental science undertaken at national facilities, working across the physical and materials sciences. This would include considering how FAIR data can be propagated across the research lifecycle, what policies, tools, and practices would support the generation and use of FAIR data, and the role of data management planning.

EnzymeML: F.A.I.R. data management in biocatalysis

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Key Words: *enzyme catalysis, standardization, reproducibility*

Enzyme catalysis provides a powerful toolbox for novel, sustainable synthesis routes and innovative solutions for bio-based chemistry. A comprehensive biochemical characterization of the desired enzyme-catalyzed reaction is essential and provides the basis for enzyme engineering and process development. Standardization of reporting of enzymatic data and metadata is considered as pivotal to accelerating bioprocess development and reducing costs. Meta-research studies suggest the lack of standardization to report and share experimental protocols, results, and data as one of the causes of the reproducibility crisis in the biomedical sciences. As first steps for the standardized reporting of enzyme function data, the enzymology and biocatalysis community has established the Standards for Reporting Enzymology Data (STRENDA) Guidelines, the STRENDA DB as a public database to make enzymatic data findable and accessible, and the XML–based data exchange format EnzymeML to make enzymatic data interoperable and reusable. An Application Programming Interface facilitates the integration of applications such as electronic lab notebooks, modelling platforms, or databases. Thus, EnzymeML enables a reproducible and scalable documentation of biocatalytic data according to the F.A.I.R. principles.

INTERCONNECTING DATA REPOSITORIES: THE PLATFORM MATERIAL*DIGITAL* (BMBF)

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Key Words: *Material data management, Standardization, Interoperability, Ontology, Workflow environments.*

Funded by the German Federal Ministry of Education and Research (BMBF), the Platform Material*Digital* aims at the development of a sustainable platform that brings together and supports interested parties from industry and academia in the digital transformation of Materials Science and Engineering [1]. This joint project between the Fraunhofer Institute for Mechanics of Materials (IWM), the Karlsruhe Institute for Technology (KIT, a member of the Helmholtz Association), the Leibniz Institute for Materials Engineering (IWT), the Max-Planck-Institut für Eisenforschung (MPIE) and the Bundesanstalt für Materialforschung und -prüfung (BAM) will develop initial approaches for the necessary complex data management, including contributions from all sectors working with materials data, such as companies, non-university research institutes and universities. By implementing this concept, a standardized exchange of data, knowledge and tools for the digitalization of materials that functions across domain boundaries is to be achieved.

In the second phase of this initiative different research projects start currently (https://www.materialdigital.de/projects/); each of these projects aims at the digital description of the complete cycle from the design to the production and characterization of a specific material – in a broad spectrum from high strength flat steels over inorganic glasses to Heusler alloys for magnetocaloric applications. In the subsequent phases of the initiative the materials data space will be progressively covered in similar projects with different funding sources.

Data-driven procedures in materials research will benefit enormously from the use of data from different sources. Their combination requires a standardization of data formats, machine-readable metadata, and the extracted information. In view of the abundance of different data sources and their broadness, a specific structuring of the data and associated metadata and information must be developed by the respective domain experts. In order to be able to take international advances in materials research and the internationally fragmented value chains in industry into account, a worldwide exchangeability and interconnectivity - interoperability - is necessary. The approach for ontology and standardization of the description of material data will be compatible with multinational initiatives such as the European Materials Modelling Council (EMMC) right from the very beginning.

The Material*Digital* platform will coordinate and advance the development of standardized software tools for the generation, storage, management, analysis, and distribution of material data. The objective of these activities is to provide both data and service providers and industrial users with a standardized, flexible, and easy-to-use toolbox for implementing digitalization projects. The development of these tools considers the wide range of material science questions, the multitude of available data sources and simulation and analysis methods, but also the dynamic development of the field. In order to enable their inclusion in industrial processes, the

interests of industrial users with regard to the confidentiality and security of their data and queries are already taken into account in the design of the tools.

In its initial version the Platform will provide two workflow environments called "pyiron" and "SimStack" in order to establish digital workflows - decentralized data or simulation concepts - by active agents within its software environment.

pyiron [2, 3] is a Python based framework which provides all the tools needed to interactively explore, implement, and run complex simulation protocols that require to combine different computer codes and to run thousands of separate calculations on high-performance computer clusters. pyiron allows to interactively implement and test simulation protocols and to upscale them for high-throughput simulations on large computer clusters.

SimStack [4] facilitates the efficient implementation, adoption and execution of complex and extensive simulation workflows and enables fast uptake of modelling techniques for advanced materials by industry. Software and workflow developers can incorporate their modules into SimStack, providing automatically generated graphical user interface for complex scientific code to the end-user.

With regard to the sustainability of the overall initiative, the Platform distinguishes between tasks that can be implemented in projects of stakeholders of different constellations and structural key and service tasks that, as enablers, should promote and accelerate the implementation of the projects in a standardized environment. On the basis of a holistic concept that includes both structuring elements and tools, the Platform develops a sustainable business model for the economic connectivity of the platform beyond the funding period.

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Building federated FAIR Data Spaces

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Key Words: *FAIR, EOSC, Semantic artefacts, Data Space*

FAIR principles (Wilkinson et al., 2016) are offering a set of generic principles supporting better research data management and data stewardship to improve Findability, Accessibility, Interoperability and Reusability of research data. Despite the international consensus around these principles a lot of practical questions still remain regarding their implementation in practice. This presentation introduces innovations proposed by EOSC related projects mainly EOSC-Pillar[1] and FAIRsFAIR[2]. These two projects are addressing the following specific questions: how can we build a service architecture that would support the aggregation and FAIRification of distributed and heterogeneous data resources? How can we make semantic artefacts FAIR to leverage the wealth of existing semantic artefacts to improve FAIRness of data?

In particular, we will present the federated FAIR Data Space service architecture currently developed in the context of EOSC Pillar. This architecture leverages and integrates existing services supporting FAIRification developed in the context of other project such as FAIRsFAIR, EOSC-Hub[3] or proposed by the GOFAIR initiative[4]. We will briefly discuss the ongoing effort in FAIRsFAIR to build recommendations for FAIR Semantics which aims at providing a common framework to build a harmonized semantic space available to enrich data content and how it will be integrated in the context of the federated FAIR Data Space.

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Development and Evolution of Materials Modelling Software

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Key Words: *Materials Modelling, Software, Research, Teaching*

Traditionally, academic codes tend to be made freely available for non-profit research as command-line software and left for commercial companies to exploit opportunities to make more accessible for industry via user-friendly interfaces and provision of support. With the increase in computing power and therefore the number of jobs, or simulations, that can be run, academics find themselves developing software to run their simulation software and collate their data and, in doing so, find they are also evolving user-friendly software. I will give an overview of the software employed in molecular and materials modelling I have helped developed and used in both in research and teaching within academia.

Addressing Industrial Needs for Atomistic Simulations through OpenKIM

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Key Words: *molecular dynamics, multiscale modelling, simulation, interatomic potentials*

Atomistic and multiscale simulations using empirical interatomic potentials (IPs) promise to address real-world industrial needs by reaching technologically-relevant length and time scales. This is particularly true with recent developments of high-accuracy machine learning IPs. However, to be trusted in industry, atomistic simulations must be reliable both in their predictive ability and reproducibility. These issues are addressed by the Open Knowledgebase of Interatomic Models project (https://openkim.org) [1-2]. OpenKIM curates IPs with full provenance control, issues them DOIs so that they can be cited in publications and retrieved for reproducibility needs, ensures their coding correctness using "Verification Checks," and tests them exhaustively using "KIM Tests" that compute a host of material properties. OpenKIM is integrated into major simulation packages (including ASE, DL_POLY, GULP, LAMMPS, and Quasicontinuum) allowing users to seamlessly use OpenKIM IPs and query their predictions (stored on openkim.org) in simulation pre- and post-processing steps.

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BUILDING A MATERIALS ENGINEERING SOFTWARE PRODUCT: FROM ACADEMIC RESEARCH TO COMMERCIALIZATION

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Key Words: *Materials Engineering, Multiscale Modelling, Software Commercialization, Innovation.*

During my undergraduate studies, I was amazed by innovative products, especially software products, and wanted to pursue a path where I could somehow advance the field of engineering through innovative approaches and technologies. In my graduate studies, I was presented to the theory of viscoelasticity and multiscale modeling techniques by my academic supervisors at Universidade Federal do Ceara (Brazil) and University of Nebraska-Lincoln (USA). At that point, I recognized an opportunity to further develop the theory and eventually build a software product that could fill the gap of existing finite element software when it comes to modeling advanced materials including highly heterogeneous viscoelastic media, e.g. fiber-reinforced thermosets and thermoplastics composites. In this presentation, I will outline the path to developing a software product based on knowledge built through academic research and founding the startup MultiMechanics Inc. With a growing team, we embarked on a path to build a valuable solution to accelerate innovation and adoption of advanced materials, while partnering with customers and industrial players to further mature and commercialize the product centered on TRUE Multiscale technology for a wide range of material-driven applications. The latest step has been the M&A with Siemens Digital Industries Software, through which our team has become the foundation of a new product line – Simcenter 3D Materials Engineering.

Scenarios for Industrial Decision Making

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Key Words: *Decision support, Multi-Objective Optimization, Industry, Business*

The activity of science is mainly about generating understanding with the aim to predict observations.[1] The formulation of the acquired knowledge in mathematical constructs makes this possible. Over the last three decades digitalisation has enabled sorting out big data sets, their fast analysis, and the simulation of possible scenarios with a predictive outcome. In addition, the requirement of causality has become less important in favour of relations that predict a certain verified reality. Business on the other hand is an economic activity still and mostly based on and driven by 19th century theory including pseudo-science mathematics complemented with after the fact explanations of failures.[2], [3] Therefore it is timely that businesses benefit from and make use of the available scientific knowledge and digitalisation tools, without getting into the fallacy that much more data supports better decision making.
For many companies, achieving the objective of a sustainable operation in a carbon neutral economy by 2050 as outlined in the European Green Deal [4] requires business decision support systems that are capable of handling not only economic but equally environmental and societal aspects of doing business. This system thinking approach will be essential to progress for meaningful decision making, but equally implies being able to deal with complex adaptive systems. Several scenarios can be considered for modelling and implementing such support systems in which the complexity depends on the operation level desired. Companies typically produce products and are integrated in a value chain, which in turn is part of a multi-value-chain network that make up a socio-economic fabric that functions within the constraints of the environment and the ecological system. Therefore, depending on the scope and ambition of the company, systems can be developed to consider the life cycle thinking, i.e., a triple P [5]– people, profit, planet – support system, at the product level, product portfolio level, value chain level, and the value chain as part of the multi-value-chain network level. In essence a hierarchy of systems can be envisaged. The implied modelling includes multi-objective optimizations [6] in combination with big data analysis on potential customers or markets and all tailored to an important business model objective. As an example, at a product level this objective could be the ecological footprint minimization of a product with an economically viable cost. In addition, the technological feasibility for the product's ecodesign options can be included.[7]
In brief, industrial business decision making can be upgraded by considering a system approach, which combines economic, environmental and societal knowledge. By taking advantage of the scientific modelling principles, the latest digital algorithms for data analysis, and digital infrastructure far more realistic actionable scenarios can be developed to set companies on track towards a sustainable future. Such business decision support systems then guide companies to become more effective in finding resolutions for coping with an ever more complex business environment.

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Ecosystem of a Software Owner towards Translation in Materials Engineering

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Key Words: *Materials Engineering, 3D Simulation, Translation, Research, Collaboration.*

Materials are everywhere… new materials are being introduced into the market at unprecedented speed. Nearly 70% of product innovation relates to material innovation. This can be the formulation of a new chemical, the new combination of existing materials, the enhancement of an available material, or a new manufacturing method as additive manufacturing. For industrial product manufacturers, materials innovation is critical for improving performance, improving recyclability and reducing cost of products. A big challenge is the amount of physical testing required to develop and certify new materials. This underlines a clear need to design materials virtually, and to validate their performance as part of complex products virtually.

As Software Owner, Siemens Digital Industries Software (DI SW) offers Simcenter 3D, a comprehensive, fully-integrated CAE solution for complex, multidisciplinary product performance engineering. The product line Simcenter 3D Materials Engineering is developed in strong connection to an Ecosystem for Materials Innovation. Our long-term connections to industrial end user customers allow us to study the right problems: we are informed about new materials questions, and we translate them into emerging needs in modelling, simulation and validation of complex material systems. We are keen on answering these questions with product innovations, and able to do so together with the other actors in the Ecosystem. Together with our top university partners, we connect to the industrial end users to fully understand their problems. The universities then drive the research into achieving the best methods to solve the industrial problem. Siemens DI SW aims to include methodology innovations into new software solutions that address the end user problem within the industrial engineering context. Siemens DI SW actively sets up and coordinates research programs and projects across the Ecosystem, involving universities, research centers, complementary technology companies and industrial end users. The broad spectrum of actors accelerates the innovation, allowing all partners to advance in their domain, overcoming the challenges together. Industrial PhD programs are an important innovation driver, thanks to the follow-up by multiple actors, and furthermore by recruiting new knowledge and skills profiles into the Ecosystem, and by strengthening the collaboration.

This presentation will outline recent technology innovations related to Simcenter 3D Materials Engineering, driven by end user needs, enabled by in-house R&D and extensions of the product offering, and empowered by strategic academic research and specialist domain-specific business collaborations. This includes advances in multiscale computational methodology, linking manufacturing simulation into the performance engineering loop, material and chemicals informatics and the strategic extension to address also the process industry.

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Title: A business model for Translation based on open source software

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Key Words: *independent translation process, open-source software*

ABSTRACT

The presentation aims to draw inspiration and ideas for a business model for independent translators by taking a closer look at the services offered by Wikki, an open-source software and consultancy company delivering services around OpenFOAM® and foam-extend.
The presentation starts with a brief introduction of Wikki and the services it offers.
As an illustrative example, the simulation of a complex heat exchanger will be outlined. The example will be used to identify where and when Wikki performs steps of a translation process (with reference to the translators' guide) and how open-source source helps Wikki to act more independently in this role.

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TOOLS FOR THE MERGE OF BUSINESS ECONOMICS, TRANSLATION AND DECISION SYSTEMS FOR SIMULATION

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Key Words: *Simulation Coaching Technical Translation Decision Systems Ontology-based Tools*

ABSTRACT

To further the industrial impact of simulation the goal of the EMMC is to provide guidance to companies. This guidance has to go beyond technical translation of one user case towards one simulation.

This guidance should bring awareness of business opportunities to all levels of company management and this guidance has to be able to create a neutral comparison between all possible options.

This talk will present the initial steps towards two tools that a COACH giving this guidance to companies can use and it will present the next tool development steps needed. The talk will end with a cordial invitation to share your knowledge on these issues.

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Implementation Strategy of the EMMC Roadmap

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Key Words: *materials, modelling, digitalisation, software development, deployment, industrial value, strategies*

The EMMC Roadmap seeks to enhance the value of materials modelling and digitalisation in Europe by increasing the industrial benefits derived from these technologies. Based on this Roadmap, which is the result of information gathering, expert meetings, and analysis by the EMMC during more than five years, this talk will highlight the results of this work by addressing key issues related to (i) the development of tools, (ii) making the tools accessible, and (iii) creating value through their exploitation. Implementation strategies for each of these points will be presented, considering scientific/technological, managerial/economic and societal/human aspects. Progress in computational materials research as well as in data sciences has been impressive, but its successful conversion into industrial values requires numerous steps. Besides the availability of high-quality interoperable software tools, one of the most critical factors is the development and training of scientists and engineers who can translate complex industrial problems into modelling strategies and communicate the computational results in a form that supports business decisions and sustainable innovation. Specific recommendations made to this end in the Roadmap will be presented, thus setting the stage for subsequent discussions.

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Demonstrating Impact

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Key Words: *Roadmap, implementation and impact, H2020, quantitative assessment*

Since its inception in 2012, the European Materials Modelling Council has generated and maintained a Roadmap [1] to address the gaps and actions raised by industry and academic partners. It has been an influential tool for policy makers and funding agencies, notably H2020 where its recommendations were adopted across several calls.

The roadmap is now in a mature state and needs continual update to respond to a dynamic global market and circumstances (such as covid-19), to reach wider audiences beyond the European frameworks, and to expand input from increasingly diverse industrial sectors.

To continue to gain influence, demonstrating the Roadmap strategy and how its implementation leads to success for industry and academia is key. Gaining feedback on qualitative and quantitative business-related impacts can be challenging as progress in new areas often requires confidentiality. In a recent, brief survey with H2020 project coordinators working on EMMC related topics, the overlaps in ambition and achieved benefits for industry points to similar goals which can be brought together for a harmonized impact statement.

In this talk and discussion, we will review the roadmap implementation strategy as it relates to H2020 ongoing project outcomes (2020-2025), discuss the common qualitative and quantitative impact strategies, relay new gaps and actions as proposed by project coordinators, and open the discussion to the audience to explore proposals to track the progress and harmonize impact statements.

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Materials Modelling and Digitalisation: a core technology in a post-COVID world

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Key Words: *COVID, Materials Modelling, Digitalisation, Sustainability, Society*

The COVID pandemic has highlighted and amplified shortcomings as well as strengths of modern society: its vulnerabilities to disruption of a world with global interactions and supply chains on the one hand and its ability to adapt quickly and offer solutions in response to the challenge on the other hand. Our way of working had to change as a result and there are likely to be long lasting transformations ahead. The pandemic has also reinforced the urgency and desire to address sustainability challenges and put even greater emphasis on the actions outlined e.g. in the European Green Deal.

These developments are set to continue. The longer society is subject to pandemic control measures, the more digitalisation is expected to grow, and the more important digitalisation will become for companies and society. Both individuals and organisations have come to realise the benefits and opportunities of a more digitally connected and digitally driven world, reducing the need to physical travel, saving time and resource on commuting and in many cases the ability to carry out substantial work for example in R&D by means of a computational, model-based approach.

In all of these aspects, materials and our ability to understand and utilise their behaviour play a central role. Below, we elaborate some key points that underline the strategic importance of materials modelling and digitalisation as key enablers of solutions to societal challenges in European post-COVID society.

https://emmc.eu/news/emmc-covid-19-statement/

A View from Academia: the Longest-term Perspective?

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Key Words: *Electronic structure*

The ONETEP code [1] is a software package that enables large-scale first-principles electronic structure calculations of real materials as a result of some distinctive features including the *in situ* optimisation of a set of local orbitals in terms of a basis set equivalent to a set of plane-waves. This talk will reflect on the experience of engagement with industry at an unusually early stage of development, including an element of co-design of functionality to meet the needs of industrial users that evolved into a partnership that has lasted over 15 years.

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Next Generation Computing @ BASF

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Key Words: *Digitalisation, Quantum Computing, Chemical Inudstry.*

ABSTRACT

Next generation computing technologies will change the way in which we approach science and business. Technologies such as quantum computing and neuromorphic computing are a quickly developing across suppliers, corporates and government. While most next generation technologies are still developing toward viable commercial applications, the promise of these technologies is enormous. Join me as I discuss the promising areas in which next generation computing can be applied.

The future, designed by materials modeling - A specialty chemicals perspective

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Key Words: *Enterprise Solutions, Specialty Chemicals, Future Perspectives*

The specialty chemicals industry is constantly striving for innovation. However, developing new solutions is becoming increasingly challenging, increased use of sustainable materials, new feedstocks derived from recycled materials, the higher need for customized solutions, or the demand for shorter innovation times, are only just a few of the challenges that must be overcome. Additionally, the specialty chemicals industry often plays an important role in providing enabling technologies, for example supporting circular plastics ecosystems by delivering tailormade materials, additives, or functional fillers.

Digitalization is a key enabler to support the industry in these current challenges; with data- and physics-based material modelling as drivers. Materials modelling – and computational chemistry in particular – has served as a helping hand in materials innovation for a long time; but mainly as a research tool, understood and used only by a few experts per company. Commonly, the lab researcher has to overcome extreme challenges to establish modelling as a part of their research workflows.

We envision a future in which materials modelling finally evolves into a tool for the many – by enabling our (lab) researchers to make use of state-of-the-art technologies without being stopped by expert-level details. Platform approaches, validated simulation workflows, enhanced user experience, and rigid uncertainty quantification are some of the key components we identify as needs for future developments.

With this impulse presentation, we want to trigger the discussion to which extent and in which time frame this could be achieved.

Benchmark of R&I programmes with the EMMC roadmap priorities

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Key Words: *Policy, Funding, Horizon Europe, Advanced Materials, MFF*

Advanced Materials and Materials Modelling are key enablers to contribute to the EU industrial competitiveness and to reach the EC policy goals, such as the Green Deal, the digitisation and the EU sovereignty.

There will be several funding opportunities spread in the different European R&I programmes currently under preparation for the next multiannual financial framework (MFF), that will help release the potential of materials modelling and digitalisation.

A general overview of the main possibilities to implement the EMMC roadmap distributed in the programmes will be presented.

The talk will set the session scene. It will be followed by programme-specific talks providing a deeper understanding of some of the programmes.

Towards pairing up materials modelling and characterisation

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Key Words: *Manufacturing, Characterisation, Modelling, Sustainability*

The future of European industrial manufacturing requires further advances in characterisation methods and computational modelling, in order to lead the way to the reliable design of new and sustainable materials and processes, rapid upscaling, and effective quality control.

These advances can only be achieved through the development of innovative techniques and a new generation of instrumentation, responding to industrial needs. These advances will be covered in this presentation.

Advanced Materials research and development in the European Defence Fund

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Key Words: *Advanced materials, European Defence Fund (EDF)*

The European Defence Fund is a new funding programme launched on 1 January 2021, and running for 7 years with a budget close to 8 billion Euro. The Fund has as its main objective fostering the competiveness, efficiency and innovation capacity of the European defence industry. It is designed as an industrial programme aiming at deepening cooperation between all defence R&D stakeholders. The main funding mechanism are grants supporting joint projects retained for funding following competitive calls for proposals.

Apart from support to projects in the main military domains (air – ground – naval – space – cyber), also funding of materials and components R&D for military applications is within the scope of the European Defence Fund.

The talk will present an overview of the current status of the European Defence Fund and the next steps to expect in the coming months. Some examples from the Fund's precursor programmes, the Preparatory action on Defence research and the European Defence Industrial Development Programme will be given.

Digital Europe: Path towards Exascale and Quantum Computing. Opportunities for materials modelling and digital transformation.

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Key Words: *Exascale Computing, Quantum Computing, Quantum Technologies, Materials Modelling, Digital Transformation.*

Abstract:
Next computing frontiers are essentially “exascale” and “quantum” computing.
Exascale Computing is the use of extremely powerful computers for applications across all branches of science, industry and public sectors related to modelling and simulation. Exascale Computers will be able to perform billions of billions of floating point operations per second and are an essential infrastructure for the Digital Economy and the digital transformation of society and industry.

Quantum Computers – funded on quantum mechanics principles - are able to tackle computation problems – such as integer factorization - substantially faster than ordinary computers.

The European Commission has been supporting the path towards Exascale and Quantum Computing and technologies as fundamental infrastructures for enabling the data revolution.

The presentation will expose the challenges in the European path towards Exascale and Quantum Computing, including opportunities for material modelling and simulation.

CHALLENGES IN THE SUPPLY CHAINS FOR THE GREEN TRANSITION

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Key Words: *Critical Raw Materials, Supply Chains, Energy Transition, Industrial Competitiveness.*

As attention to climate change and its effects is increasing, the European Commission has launched the European Green Deal. This ambitious plan will be the basis of the European growth strategy and will see the decarbonisation of European economies and energy systems, with a commitment to reach carbon neutrality by 2050. The realisation of the Green Deal requires a swift transition to clean energy and mobility. However, the availability of several materials key for clean technologies is a possible bottleneck. In particular, several raw materials used in clean technologies have a strategic importance and high supply risks and have thus been flagged as critical [1].

The Joint Research Centre of the European Commission is actively monitoring the current situation and studying future developments. Potential risks are assessed in four steps of the supply chains (i.e., raw and processed materials, components and assemblies) for strategic technologies [2] and specifically for clean technologies (e.g., wind turbines, solar photovoltaics, electric mobility) [3,4]. For most technologies, the raw and the processed materials steps are the most alarming. Geological resource availability, trade barriers, concentration of supplies, lack of mature and stable markets are some of the challenges identified. Moreover, demand is likely to increase significantly for all materials -critical and not- with increased competition for resources amongst different sectors and manufacturers. In the highest demand scenarios, corresponding to a high deployment of clean technologies and low materials efficiencies, projected demand of specific materials may increase between 12 and 40 times from 2018 to 2050. This presentation provides a general overview of our latest findings.

Among other actions, these challenges call for a faster development and market deployment of new products with a focus on increased material efficiency and substitution of critical materials. Advancements in material modelling could be instrumental in making this happen. Moreover, digitalisation could help improving the analysis of supply chain risks. One of the current challenges is access to reliable and updated information, especially in terms of material intensities and lifetimes of products.

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Open Contribution - Abstracts

New Modelling Approach for Edge Cracking Simulations

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KEY WORDS: EDGE CRACKING, ESSENTIAL WORK OF FRACTUE, EWF, DOBLE EDGE NOTCH TEST, DENT, FORMING SIMULATION.

The use of new high strength sheet materials still represents a challenge to the manufacturing sector. It faces serious industrial problems to reach defect-free production as well as productivity losses due to the unpredictable occurrence of edge cracking and lack of overall formability during forming.

In most of the cases, the contour or even the tool itself must be modified and sometimes, the sheet material has to be changed. This results in high additional costs and delays in part delivery programs or can even impede the manufacture of parts with high-strength materials. Traditionally, sheet formability has been addressed through tensile tests and forming limit curves (FLC), with good enough results. However, such tests do not allow understanding crack-related problems, which remain as still unsolved issues in the sector and hamper the use of new materials and the development of high-performance parts at reduced costs. Accordingly, FormPlanet addresses the urgent need for accurate material characterization tests and new modelling approaches to predict defect generation at an early design state, as well as to prevent and to solve it during industrial manufacturing, covering the whole value chain.

In this framework, a new approach to define the ductile damage model based on the toughness in terms of essential work of fracture (EWF) obtained by doble edge notched tension test [1] (DENT) is presented. This methodology allows improve the finite elements analysis (FEA) showing a good edge cracking prediction on forming operations of AHSS. Both laboratory tests and forming of industrial parts were analyzed using the proposed method.

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MODELLING STRATEGY AT THE LIGHTCOCE PROJECT: AN ECOSYSTEM FOR ADVANCED MATERIALS

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Key Words: *Multiphysics Problems, Industrial impact, translation.*

Contributions The full title of the project summarizes its objectives "Building an Ecosystem for the up-scaling of lightweight multi-functional concrete and ceramic materials and structures". LightCoce is a research H2020 project that belongs to the Open Innovation Test Beds group. During the last decades a trend towards the use of lightweight materials in constructions and infrastructures, as well as for the aerospace, automotive and defence industry has been observed. Lightweight durable components are easy to transport, handle and install and demand less operational energy reducing substantially their environmental footprint, as well as the relative costs. Among other materials, concrete and ceramics are on the focus of interest due to their wide range of applications and their durability. Based on end applications lightweight attributes must be coupled with enhanced properties and multifunctionalities. However, pilots are bulky and expensive facilities which in most of the cases require upgrades to be modular and flexible in application, while administrative burdens often delay project kick-off and funding gaps are difficult to overcome, making the majority of the already existing efforts to remain on a lab or in restricted pilot level with limited exploitation capacity for further industrialization. The main objective of the LightCoce project is to cover the gap in the upscaling and testing.

A multiscale material model methodology has been applied to correlate the material composition, structure and manufacturing process with their physical performance. Combining atomistic, coarse grained, meso finite element models and macro models, relationships between composition, porosity or volume fraction with the final mechanical, thermal, hygrothermal or self-sensing material properties have been established. In order to minimize the energy, a link between the energy consumption and the most critical industrial processes have been determined. Finally, an easy-to-use methodology to estimate the optimal materials' properties combined with minimising manufacturing energy consumption has been proposed. The methods developed consider the impacts on the cost and emissions avoided during the manufacturing process performing the multidisciplinary design optimisation (MDO) of the material. The resulting output represents the best manufacturing option to obtain the final product optimised in energy consumption and material properties.

In the coming months, Lightcoce project plans to launch an open call, inviting new cases to enter into the eco-system, and benefit of the Lightcoce project services (including modelling) free-of-charge. The proposed test cases should be in the area of lightweight, nanoenabled concrete, traditional ceramics and advanced ceramic materials and the starting TRL should be at least 4-5. The call is expected to be launched towards the end of April and more information will be available at a later date in the program web-site: www.lightcoce-oitb.eu .

IM2D: an industry-driven interoperable solution for the simulation-aided design of emerging electronics

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Key Words: *Interoperability, industry-driven software, emerging electronics.*

Contribution: The current and major worldwide drive for big data, machine learning, and quantum computing will push away from traditional all-silicon platforms, and provide a clean slate for industry to rapidly deploy novel technologies based on innovative materials and devices. This requires fast exploration of materials' properties (e.g. memory effects for memristive computing), linking materials properties to performance in unexplored architectures, and assessing their business potential. Here, we present an interoperable material-to-device simulation platform, named IM2D, for characterization and design of synaptic electronics for neuromorphic computing. IM2D conjugates the advantages of material and device-driven software, connecting the properties of materials at the atomistic level to the electrical behavior of devices, with the aim to reduce the gap between materials and device realms and sustain the simulation-aided R&D processes of semiconductor industries and SMEs. IM2D is based on the integration of first-principles materials modelling approaches and modelling software for emerging devices, fully compliant with a vision of semantic interoperability, driven by standardized ontologies. We demonstrate the capability of the IM2D software, by investigating the switching mechanisms in amorphous chalcogenide materials, proposed for non-volatile memory devices and selectors.

A beta version of IM2D is now available on request for early adopters. If interested contact us at intersect@nano.cnr.it or subscribe to our newsletter. See https://intersect-project.eu for further details and news.

This work was supported in part by EC through H2020- NMBP-TO-IND project GA n. 814487 (INTERSECT).

Surface Free Energy Characterization of Soft Materials through Computational Experiments

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ABSTRACT

The surface free energy of soft coatings determines the adhesion, friction, and wettability response of solid surfaces in several applications of engineering and biomedical interest. However, the multiscale nature of these phenomena limits a bottom-up prediction of the resulting surface properties.

In this work we use computational experiments to characterize the surface and solid-fluid interface of low-surface-free-energy coatings and materials. In particular, the free energy perturbation approach is first used to evaluate the work of adhesion between polymer surfaces and fluids; then, the Young-Dupré equation is adopted to compute the ideal contact angle. Such molecular dynamics and coarse-grained simulations allow to explore the interfacial properties of soft materials, enabling a more comprehensive understanding of their effect on the adhesion, friction, and wettability of solid surfaces. Differently from standardized experimental approaches, numerical experiments allow to understand and decouple the different mechanisms regulating the wetting properties of soft coatings with atomistic precision. The aim is to propose a first step towards a multiscale standard framework for the computational characterization of surfaces, required for the optimal design of super-hydrophobic materials.

The results obtained in this work will be used as input parameters for materials modeling at higher scales, such as finite elements simulations, to investigate the contribution of surface topology on wettability, in terms of nano- and micro-roughness or patterning. In perspective, multiscale models linking the chemical and topological characteristics of soft surfaces with their effective response will allow predictive in silico testing of new materials with tunable functionalities.

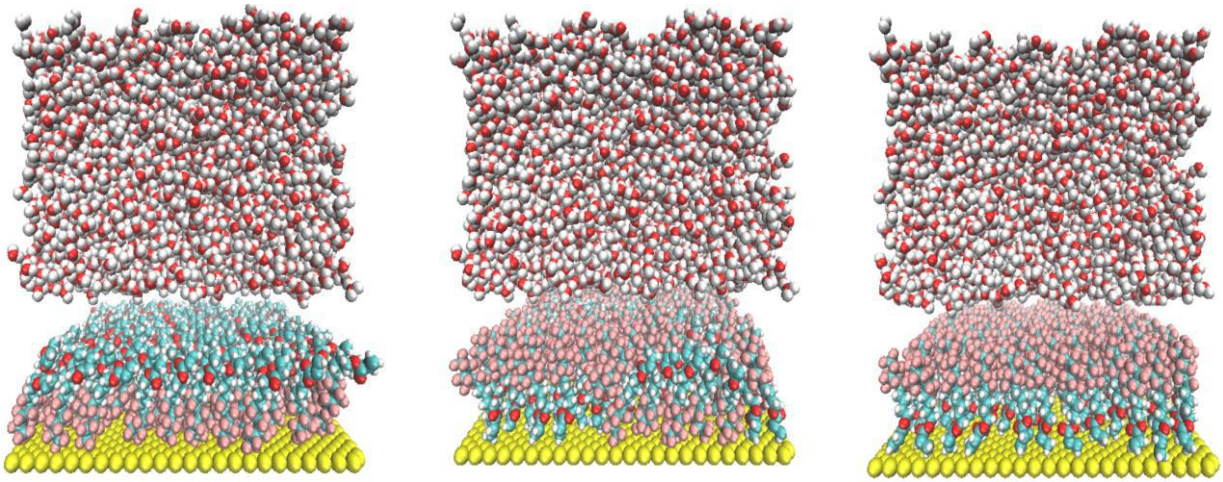

Figure 1. Different coatings of a solid surface in contact with water modelled by atomistic simulations.

A reversible coarse grained model for truly accurate multi-scale simulations

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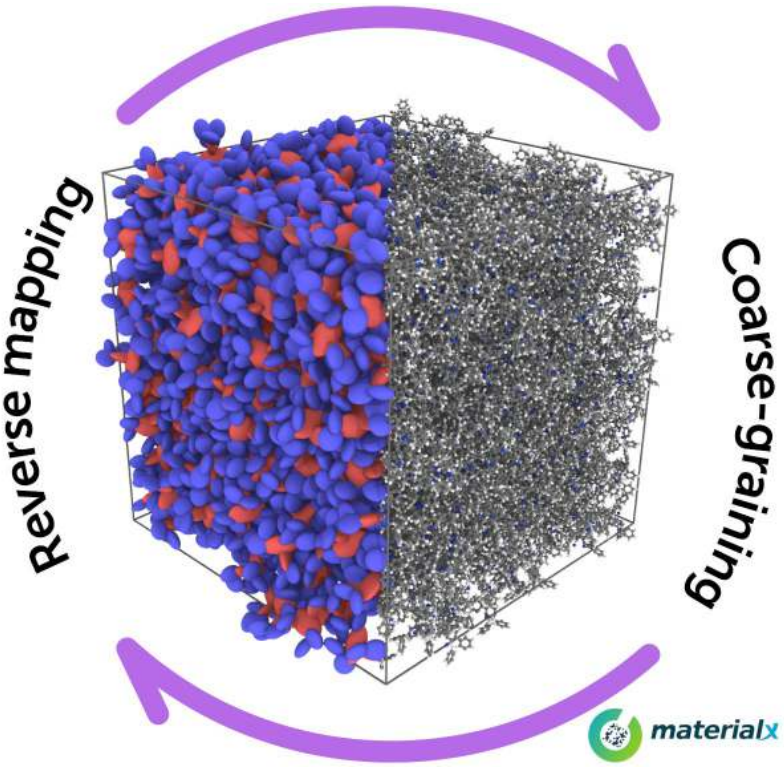
Key Words: *Coarse-grained models, Reverse-mapping, Molecular Dynamics*

An innovative coarse grained (CG) model has been recently released for the description of complex organic molecules. This model is able to describe large-scale morphology (e.g. amorphous matrices, thin-films) with a structural accuracy comparable to that of more sophisticated approaches, yet at a fraction of the computational cost and time. Unlike most CG models, the presented one has the ability to reproduce the excluded volume of molecules at a level comparable to those of atomic force fields. This unique characteristic allows the reverse-mapping of atomic coordinates which are suitable to carry out electronic-structure calculations, capturing the complexity of real materials. The general characteristics, advantages and trade-offs of the model are presented, along with a selection of case studies in the field of organic electronics.



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Towards a Microstructure Simulation Ecosystem

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Key Words: *microstructure simulation, interoperability, simulation platforms, microstructure ontology, processing-microstructure relationship*

The microstructure is the state variables determining the properties of any material and accordingly also of any component made from a material. The simulation of microstructure evolution even in complex metallic alloys has made enormous progress in the last decade. Respective simulation tools like MICRESS® [1] meanwhile are successfully used to tackle and to solve problems of industrial interest [2],[3],[4].
Microstructure evolution occurs at the boundary between processes occurring at the macroscopic scale of the component and the atomistic scale determining e.g. the properties of pure phases or the properties of interfaces. Microstructures further integrate all effects and phenomena occurring along the entire processing history of a component. Simulating the evolution of microstructures thus requires interoperability between a variety of simulation codes operating at different scales and also a seamless data exchange between experimental microstructure data and their simulated counterparts [5] as well as thermodynamic and kinetic data. This variety of tools and data eventually has to be orchestrated by suitable tools. Modular configurable workflows eventually must be executed on suitable grid-based platforms [6] or in a cloud-based infrastructure [7].
The information exchange within such an ecosystem must be based on format and data standards or even better on an ontology. The development of a microstructure ontology e.g. based on a first metadata description [8] is objective of a recent task group of the EMMC.

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Computer Aided Design of OLED Materials – multi-scale modeling

Software for Chemistry & Materials[1] + Simbeyond[2]

(Presented by T.P.M. Goumans and A. Vauzelle)

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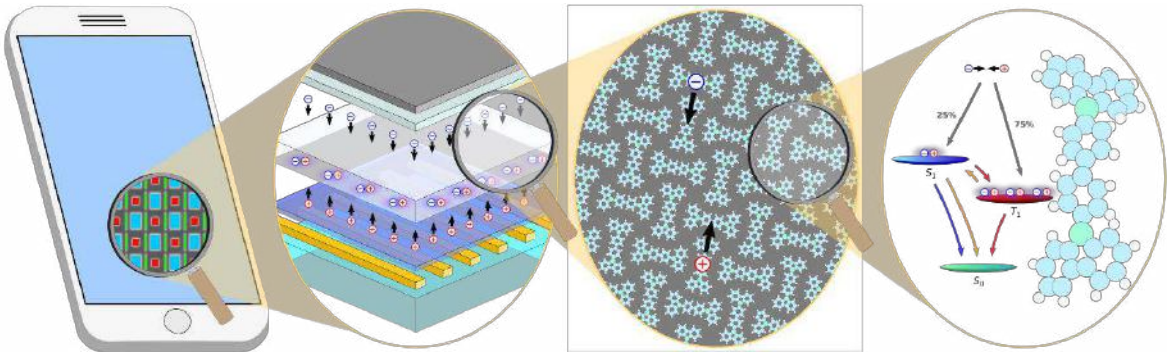
Key Words: *Multi-scale modeling, software and model development, industrial applications, organic electronics, OLEDs.*

The behavior of materials, components, and therefore entire devices are ultimately determined at an atomistic level. Computational modeling can be used to predict and understand the properties of materials from an atomistic bottom-up approach. Through insight and predictive calculations the most suitable materials for a certain purpose can be selected from a large pool of candidates, reducing the time and resources to develop new and better polymers, batteries, computer chips, and organic electronic devices.

We demonstrate how industry has been using quantum chemistry to model charge transport[1,2] and luminescence properties[3,4] to predict and optimize new OLED materials. On the other end of the simulation scale, simulations of optoelectronic processes in disordered materials are necessary to predict the electrical characteristics, efficiency, color point, and lifetime of full devices[5],[6]. A brand-new collaboration between SCM and Simbeyond will develop the first fully integrated multi-scale simulation pipeline for OLEDs, marrying the Amsterdam Modeling Suite with Bumblebee. Such a user-friendly modeling platform will further reduce the development costs for new and improved OLEDs.



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BattINFO: The ontology for the Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)

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Key Words: *Battery, Electrochemistry, Interoperability, Digitalization, Ontology*

The Battery Interface Ontology (BattINFO) is an ontology of batteries and their interfaces developed for the Battery Interface Genome – Materials Acceleration Platform project (BIG-MAP) and BATTERY 2030+, which is based on the top-level European Materials and Modelling Ontology (EMMO) [1].

BattINFO [2] aims to formalize the current state of knowledge on battery interfaces to support the development of computational tools and the deployment of interoperable data in the BIG-MAP project and beyond. The definitions included in BattINFO are based as far as possible on accepted standards defined by the International Union of Pure and Applied Chemistry (IUPAC) or other preeminent textbooks on the subject. BattINFO classes and their relations to each other are designed with three goals in mind: (i) to be scientifically rigorous and accurate, (ii) to reflect current battery orthodoxy and dominant jargon, and (iii) to be flexible to describe a range of battery chemistries, not only Li-ion.

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DATA-LED STRUCTURE ANALYSIS OF SIMPLE AND MULICOMPONENT CARBIDES AND PHASE NUCLEATION

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Key Words: First Principles Calculations; *Multicomponent Carbides; Anisotropy, Nucleation.*

Abstract: The ground state structural and property data of different carbide systems (simple carbides (e.g. MC_x), multicomponent carbides (e.g. $(Fe,M)_7C_3$), where M represents different alloying elements (Ti, V, Nb, Cr, etc.)) are important for material development and processing. Carbides of complex compositions are widely used in key engineering ceramics and manufacturing tools as well as existing as secondary particles in various complex alloys. The structure and properties of secondary carbides directly affect the stiffness, strength, hardness, thermal conductivities and toughness of the alloys. The structural parameters of secondary phases also influence the nucleation and growth of metallic phases or other phases of different melting points (e.g. Ferrite, Austenite, M_7C_3, in steels and wear resistant welded hardfacings). Development of systematic structural data (e.g. lattice parameters, anisotropy) and the dependence of lattice characteristics on doping elements/defects in the crystals are important research areas supported by rapid development of computational tools. It will provide data for the predictive analysis on the effectiveness of secondary particle as nucleation sites for other metallic or ceramic phases.

In this work, as part of a main project, in developing data led approach in advanced welding structures of complex alloying systems, first principle calculation and python program based data analysis is combined to establish systematic data of simple carbides (MC_x and $M(C, N)_x$) and multicomponent carbides (M_7C_3). A python program is developed to analysis systematic data of functional structural characteristics and lattice misfit data between different crystals based on Atomic Simulation Environment (ASE) and Crystallographic Files of different format.

The work shows that the combine approach can effectively develop deep data linking lattice data to functional properties and material behaviours in manufacturing. Typical lattice misfit and energy analysis data reflecting the effectiveness of a compound as a nucleation site for another phase is presented and compared with data from previous works based on empirical approaches. The effect of different alloying elements (including rare earth (RE) elements) on the crystal structures of multicomponent carbides is studied. The doping elements showed different effects on the lattice parameters of MC_x/$M(C,N)_x$ and their effectiveness as nucleation sites for other low melting point phases. The use of the physical modelling data in composition design and development for enhanced functional properties in carbide based welded hardfacings and other systems is discussed.

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EMMO-python - working with EMMO in python.

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Key Words: *EMMO, Interoperability, Ontology-tools, Python, Emmopython*

EMMO-python [1] is a Python API for the European Materials & Modelling Ontology (EMMO) [2]. The package is built on top of Owlready2 [3], a python package with extensive support for ontology development and usage. EMMO-python has developed organically with EMMO, and a set of tools intended for easier development and documentation of (EMMO-based) ontologies has been created:

- **ontoversion** returns the version of the given ontology based on the version IRI.
- **ontoconvert** enables conversion between different formats for the ontology. This is particularly useful for converting between the turtle (.ttl) and rdf/xml (.owl) formats. An option for reasoning the ontology with Fact++ is included, e.g. reasoning can be done directly from the command line.
- **ontograph** makes graphs of the ontology. Leafs and roots can be specified so that only the desired parts of the ontology are included in the Figure. Furthermore, module-interdependencies can be plotted instead of their content.
- **ontodoc** is a tool to document your ontology. It will generate a minimal documentation without arguments, but options for format as well as content templates are available.
- **emmocheck** is a particularly useful tool during development of ontologies based on EMMO. This tool checks that the given ontology conforms to the conventions of EMMO.

Several options are available for these tools, and we refer to the documentation [4] for complete instructions.

In this interactive session small examples on the use of the tools as well as some demo-examples on possible usage will be presented.

EMMO-python is packaged and available through pypi [5] for easy installation. Also, a Dockerfile is made available for easier installation with regards to dependencies, particularly graphviz, pandoc and pdflatex, required for the documentation and generation of figures. EMMO-python is an ongoing effort, adapting to the developments in EMMO. New features are being added when the need has been identified. Contributions and suggestions are very welcome and may be opened on the github repository.

We propose the formation of an EMMC Task group: 'Tools for working with ontologies', within the EMMC focus area 'Interoperability', and we welcome discussions on the formation and interest for such a group during this interactive session.

Contributions to EMMO-python and examples of use are from the following projects funded through the European Union's Horizon 2020 research and innovation programme: EMMC-CSA (#723867), Marketplace (#760173), OntoTrans (# 862136), OntoCommons (#958371), BIGMAP (# 957189). Furthermore, EMMO-python is used in SFI PhysMet (Norwegian research council #309584).

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MDO - An Ontology for the Materials Design Domain

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Key Words: *Ontology, Materials science.*

In the materials design domain, much of the data from materials calculations are stored in different heterogeneous databases. Materials databases usually have different data models. Therefore, the users have to face the challenges to find the data from adequate sources and integrate data from multiple sources.
Ontologies and ontology-based techniques can address such problems as the formal representation of domain knowledge can make data more available and interoperable among different systems. In this poster, we introduce the Materials Design Ontology (MDO), which defines concepts and relations to cover knowledge in the field of materials design. MDO is designed using domain knowledge in materials science (especially in solid-state physics), and is guided by the data from several databases in the materials design field.
We show the application of MDO to materials data retrieved from well-known materials databases.

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OntoCommons
Ontology-driven data documentation for Industry Commons

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Key Words: *strandardised data documentation, ontology, interoperability of data, FAIR data, demonstrators on use of ontologies, networking and cooparation, coordination and support actions.*

ABSTRACT

OntoCommons lays the foundation for interoperable and standardised data documentation across all materials and manufacturing domains, thereby facilitating data sharing and pushing data-driven innovation to bring out a truly Digital Single Market and new business models for European industry to meet the opportunities of digitalisation and sustainability challenges.

This will be achieved by coordinating a wide range of EU stakeholders for the development of an Ontology Commons EcoSystem (OCES) that comprises a set of ontologies and tools following specific standardisation rules. OCES provides a sustainable approach to harmonised data documentation through ontologies, making the data FAIR (Findable, Accessible, Interoperable and Reusable), and implementing practical and user-friendly mechanisms of intra- and cross-domain interoperability focusing on materials and manufacturing sectors. Demonstration cases with strong industrial involvement covering a wide range of NMBP application domains and stakeholders' feedback loops will guide the OCES development to prove its effectiveness in accelerating data-driven innovation.

OntoCommons represents relevant stakeholder knowledge by bringing together a consortium from a wide range of communities, including subject-matter experts (e.g. material scientists), ontologists (e.g. philosophers, semantic web experts), implementers (e.g. database experts), industrial end users (e.g. manufacturers), and application developers.

OntoCommons will achieve its aims through activities consistent with its CSA nature, building on communication, networking, coordination and cooperation between EU and international stakeholders connected with relevant National, European and international projects, initiatives and bodies (incl standards organisations) facilitating the access to the available state of the art and emerging tools and solutions as well as the harmonisation of already existing EU funded initiatives, making efficient use of EU resources.

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OntoTrans
Ontology driven Open Translation Environment

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Key Words: *Open Translation Environment, Materials Ontology, Artificial Intelligence, Materials Modelling Solutions, Modelling Workflows, Open Simulation Platform, Materials and Process Design, Semantic Systems*

ABSTRACT

OntoTrans provides an ontology-based Open Translation Environment. Its Artificial Intelligence approach enables end users to represent in a standard ontological form their manufacturing process challenges and to connect them with relevant information sources and materials modelling solutions, capable to support optimal materials and process design.

OntoTrans provides smart targeted guidance through the whole translation process, namely from the initial user case specification to actual materials modelling workflows with related validation, verification and uncertainty quantifications to deliver a full complete experience to companies. This is achieved via analysis of available data (data fusion), modelling workflow options, simulation and contextual results interpretation.

OntoTrans is fully integrated into existing and emerging developments in materials and manufacturing, including integration with digital materials modelling marketplaces and open simulation platforms. It's footing on the European Materials Modelling Ontology (EMMO) ensuring wide interoperability and standardisation.

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https://ontotrans.eu/

A PHYSICS-GUIDED MACHINE LEARNING MODEL BASED ON PERIDYNAMICS

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Key Words: *Peridynamics, machine learning, fracture, physics-guided.*

With the rapid growth of available data and computing resources, using data-driven models is a potential approach in many scientific disciplines and engineering. However, for complex physical phenomena that have limited data, the data-driven models are lacking robustness and fail to provide good predictions. Theory-guided data science is the recent technology that can take advantage of both physics-driven and data-driven models. In this presentation, a new physics-guided machine learning model based on peridynamics will be presented [1,2]. Peridynamics is a suitable approach for predicting progressive damages because the theory uses integro-differential equations instead of partial differential equations. Several numerical examples will be shown to demonstrate the capability of the methodology.

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Predicting the properties of molecular materials: multiscale simulation workflows meet machine learning

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Key Words: *Multiscale Modelling, Workflows, Ontology, Artificial Intelligence, Machine Learning.*

In recent years, machine learning (ML) methods have applied with success to studies of the properties of molecular materials. The vast majority of these studies are focused on the properties of individual molecules, targeting the correlation between molecular structure and resulting properties. The properties of several technological materials constituted by molecular aggregates, however, depend on both molecular structure and on aggregation morphology, as for example the case of nanoscale materials. Computational methods for predicting the properties of molecular materials must therefore integrate the properties of individual molecules with information about aggregation morphology, which, in turn, can be related to materials fabrication and processing. The definition of a modelling paradigm able to simulate and predict the properties of molecular materials as a function of molecular structure and aggregation/fabrication conditions can potentially enable high-throughput development of novel materials for technological applications. In this work, we design and implement a computational workflow for the simulation of the properties of molecular materials integrated with a ML scheme for enhancing the computational workload. The workflow is based on a multi-scale top-down approach, in which target properties are defined from the application to the molecular scale. The workflow is implemented through top-down hierarchical data structures, which connects the properties of molecular materials at the nanoscale to the atomistic/electronic scale. Modelling data are generated by applying domain-specific simulation protocols based on atomistic molecular dynamics and density functional theory calculations. ML approaches are therefore applied to enable the scale reduction, providing a local mapping at a lower scale of the properties of large molecular aggregates, reducing greatly the overall computational load. The proposed approach is applied to the evaluation of intermolecular electronic couplings of aggregates of organic molecular semiconductors, a key quantity for the development of materials for advanced electronics. Preliminary studies suggest the relevance of the specific set of features considered for representing intermolecular properties, which depend on the aggregation morphology. Work is in progress to assess the interplay between the structure of individual molecules and the structure of aggregates in determining the performance of ML predictions of the properties of molecular materials. Moreover, an additional speedup of the whole workflow is obtained by optimizing the implementation of the integration between the multiscale simulation workflow and the ML engine.

In order to facilitate the entire process, we started the development of an ontology materials science, with particular focus on molecular materials. The core of the projects revolves around the idea that a chemico-physical object is represented by its structural features and properties, while computational and experimental workflows are separately represented but results are 100% interoperable. We linked our work to pre-existing ontologies, like MDO and EMMO, trying to keep them as compatible as possible. Succeeding in developing this ontology should

help re-organizing the community working on molecular materials, which is a field historically filled with many different formats, procedures, and conventions. We hope to help researchers to both speed up their personal work while also making communications between different teams easier and quicker. Finally, the development of unifying standards will also serve as an incredibly powerful accelerator for the application of machine learning and all kinds of data intensive applications to materials science.

An ontology for physical metallurgy

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Key Words: *material science, ontology, interoperability.*

SFI PhysMet - Centre for Sustainable and Competitive Metallurgical and Manufacturing Industry [1] is a newly funded Norwegian centre for research-based innovation lasting from 2020 to 2028. The aim is to accelerate the transformation of the national metallurgical and manufacturing industry towards more sustainable and cost-efficient production and future material products, solutions, and improved processing methods. To integrate models and tools, an ontology dedicated to metallic alloys microstructure and properties will be developed. The ontology will be released under a creative commons license (CC-BY 4.0).

The goal is to develop an EMMO-based [2] domain ontology for microstructure and connect it to process and characterization ontologies.

This ontology dedicated to physical metallurgy will strongly focus on microstructure, defined as a “state” of a material from which properties can be extracted and which can be altered by “processes”. While focusing mostly on aluminium and ferrous alloys, this work will contribute to a more generic microstructure Domain Ontology providing a common representational language for describing microstructures of metallic and non-metallic materials (polymers, ceramics etc.), including all aspects needed to support connecting microstructure characterisation to data processing and through-scale and through process modelling by close collaboration with the EMMC task group.

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