



Candidate for Chair of the Organisational Assembly

Natalia Konchakova

Motivation

It is extremely important to narrow the gap between industrial needs and requirements and materials modelling research by generating collaborations, creating new values and knowledge together, supporting actionable evidential knowledge and decisions and by developing professional network.

The EMMC leads the integration of materials modelling in European industry and the digitalization of materials science, stimulating innovations based on materials modelling.

To increase the modelling impact in industry, effective materials modelling translation, including aspects of transparency of decision-making guided by modelling and innovation process implementation based on digitalization, should be developed. This is a major task of the EMMC focus area of Impact in Industry, which I will support and develop intensively to ensure the interests and benefits of organizations members.

As a Chair of the Organisational Assembly, I will promote interests of the organizations members in all activities of the EMMC to extend modeling integration / use by industry and support innovations.



Dr. Natalia Konchakova

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Short CV

Dr. Natalia Konchakova is a senior scientist at Helmholtz-Zentrum Hereon, Germany. She works in the fields of materials modelling, simulation and characterization of lightweight metals, computation analysis of surface degradation and failure due to aggressive environment (corrosion) and intensive mechanical loading.

In the frame of the EMMC activity, Natalia put her expertise in the Translation concept development, an open innovation platform creation and digitalization of some specific industrial relevant problems to increase the impact and industrial exploitation of materials modelling.

Natalia Konchakova is the coordinator of the H2020 project VIPCOAT "Virtual Open Innovation

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Platform for Active Protective Coatings Guided by Modelling and Optimization“, <https://ms.hereon.de/vipcoat/>, (Grant Agreement No 952903).

She is a co-author of some white papers on the EMMC related topics like Translation and Open Innovation Framework for materials modelling:

Translation in Materials Modelling – Process and Progress, <https://zenodo.org/record/4729918#.Yoqnx-xVhE>

EMMC Translators Guide, <https://zenodo.org/record/3552260#.YoqoF9-xVhE>

Position Paper: Open Innovation in Horizon Europe, <https://zenodo.org/record/5848552#.Yoqobd-xVhE>





Candidate for Chair of the Organisational Assembly

Franz Pirker

Motivation

It's all about materials - Materials are the foundation for almost all innovations and an important building block for the European Industry. Materials modelling is the key enabling technology – supporting industrial innovations. EMMC has created a visible and successful platform in the field of materials modelling. The roadmaps, industrial case studies or MODA as “accepted standard” are just some of success stories.

After two years being a Co-Chair and representing the Organisational Members in the BoD, bringing in and discussing new ideas with BoD members my personal goal (when being re-elected) is to give the organisational members a much louder voice as it is defined in the EMMS statutes.

Therefore, I defined three main goals for the future period:

- Creating additional added values for EMMC organisational members which are measurable
- Shifting the EMMC from a bottom-up organisation to a relevant stakeholder organisation representing the materials modelling ECO-system
- Pushing a direct information channel to ensure transparent information and communication in between EMMC
- With the broad expertise of the Organisational Members (different scientific and business expertise), we have the basis to establish EMMC as THE European platform representing all material modelling stakeholders.



Dipl.-Ing. Franz Pirker, MSc

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Short CV

DI Franz Pirker, MSc is business development manager at AC2T research GmbH, Austria. He is responsible for, development of new business areas, the commercialization of IPRs and software and key accounting. Additionally, he coordinates the H2020 project

i-TRIBOMAT (www.i-tribomat.eu), an Open Innovation Test Bed for tribological materials characterization and upscaling. This project aims to set up new digital services and business models combining tribological characterization and materials up-scaling via modelling and simulation.

Within EMMC Franz brings in his expertise in development and commercialization of software models and products as well as setting up digital business models.



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Ilian Todorov

Motivation

My ambition for the role is to create a better interface and feedback loop between the organisational members (OM) and focus area (FA) leads with the Board of Directors (BoD). I will challenge the EMMC BoD to improve and enhance their communication with the council membership and to provide a channel of regular updates of their work and essential highlights of value to the community.

I will work with the BoD to assist the creation and establishing of EMMC Working Groups, contributing to Value of Membership, Self-regulation (Statutes) and Knowledge Transfer (captured value proposition of materials modelling), to help bring in place more effective bottom-up operations of the EMMC ASBL.

I will work together with the FAs' groups to provide a better, more transparent and agile web-presence of their collaborative work and assets and encourage their use of transparent and easy to contribute collaborative tools for work as forum channels, GitHub and open google documents.

I will work with the OMs to define and capture their digitalisation needs and requirements from different FAs' assets. Collaboratively with FAs leads, I will help identify the sustainability factors, as barriers and incentives, across the FAs, essential for both digital assets and researchers.

I will promote the council work and vision to and look after its relationship and connections with the broader R&D communities on both the computational and experimental sides, spanning the technology innovation spectrum from scientific excellence at academia and research centres, up to materials modelling value and impact in industry.



Prof. Ilian Todorov

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Short CV

Prof. Ilian Todorov leads the Computational Chemistry group at STFC Daresbury Laboratory. With over 20 year's experience in the field of HPC software engineering for materials modelling, he has led the UK flagship MD package, DL_POLY, and researched prospective materials for used nuclear fuel encapsulation with colleagues at Bristol, Sheffield and Queen Mary, London. He is involved in a number of academic communities in the UK (CCP5, MCC, UKCOMES and RSE Society and FAIR4RS@RDA) and is partnering in the EMMC related projects VIMMP, OntoCommons and DOME4.0.

Ilian will support EMMC in bringing in his expertise and experience with best practices in research software engineering, academic and industry outreach, training and translation. [More ...](#)



Candidate for Chair of the Organisational Assembly

Jürgen Spitaler

Motivation

Novel materials are at the heart of technologies to address the major challenges of today's world such as sustainable and affordable energy, communication and transport, with large impact on economy, ecology, political stability and social welfare. The community is on the transition to a next level of materials design, which is about usage of all available knowledge and data using artificial intelligence in order to accelerate the design of new materials and processes.

In this context, the EMMC is the institution to coordinate efforts for linking, standardizing and networking, which are a key for fostering the transition to the next level of materials design. The EMMC provides an outstanding opportunity to participate actively in this transition, bringing people together and paving the way to strengthen the material modeling community in Europe.

I see the following priorities for the EMMC in the near and mid-term future:

- Continue and intensify the work on standards for data-formats, ontologies and interfaces between simulation platforms and databases.
- Create a larger number of best-practice examples for the usage of materials modeling for industrial use cases.
- Continue the successful work as a hub for networking between partners from industry, SMEs, research institutes and academia.
- Enable new members to participate in European networking and funding activities.



Dr. Jürgen Spitaler

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Candidate for Chair of the Organisational Assembly

Short CV

Dr. Jürgen Spitaler is Key Scientist Computational Materials Design at [Materials Center Leoben Forschung GmbH \(MCL\)](#), Leoben, Austria.

Since 2009 he is involved in several national and European funded projects, like

- From 04/2021 *MCacceL – Development and implementation of a materials acceleration platform at MCL (IC-MPPE Project P1.9)*, Key researcher and Operative Project Manager.
- 07/2020 – 06/2023 *POLDERS – Polarization Decorrelation Regions in Perovskite Relaxors* (since 01/202 (FWF-project I 4581-N), Key Researcher/contribution to project proposal.
- From 06/2019 CITRES – Chemistry and interface tailored lead-free relaxor thin films for energy storage capacitors (ERC consolidator grant 817190, PI Marco Deluca), Key Researcher/contribution to project proposal.

...

He also contributed to the organisation of national and international workshops like

- 09/2022 Symposium Materials Acceleration Platforms for future materials design at MSE 2022; Co-organizer.
- 10/2021 Virtual Psi-k GreenALM hands-on tutorial 2021; Main organizer.
- 10/2019 GreenALM workshop 2019; Main organizer.

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Development of codes:

- **GreenALM:** Green's function based DFT code for alloy modeling; software management.
- **SpheRaE tool:** Tool for the DFT-based prediction of full Raman of polycrystalline materials based on DFT; support for method development and software management.
- **ElaStic:** Software tool for the ab-initio calculation of elastic constants; software management, scientific supervision.
- **Exciting/Elk:** DFT code for ground state and excited states properties; project management as well as implementation of tools for visualization and the k.p method for faster band structure calculations.
- **ATAT@WIEN2k:** Interface for cluster expansion based on Wien2k; project management and support for implementation.

[More ...](#)



Candidate for Chair of the Organisational Assembly

Costas Charitidis

Motivation

Materials modelling is at the centre of the modern science. Through modeling at all scales, materials characteristics and properties can be predicted giving rise to the scientific community and the industry to open new roads in the development of advanced materials. Furthermore, materials modeling can be conducted indirectly through modeling of production processes in close connection with the so-called digitalization providing the possibility of improving the production of materials.



However, materials modeling cannot be independent from materials characterization and the interface between the two should be always under thorough consideration and discussion (through close collaboration with the EMCC cluster) since it opens numerous possibilities in new scientific fields. Considering the constant optimization of instruments and hardware many opportunities for the development of innovative and validated suites of models arise, in order to improve the impact of industrial manufacturing.

Thus, it is expected to increase the contributions towards semantics development in the domain of characterization and modelling as well. Finally, supporting the policymaking and roadmapping processes, as well as engaging more stakeholders to EMMC are anticipated as part of joining this honorable position.

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Short CV

Costas Charitidis is Professor in the School of Chemical Engineering of the National Technical University of Athens and Director of the Laboratory of Advanced, Composite, Nano Materials & Nanotechnology. He is member of the Scientific Council of the Hellenic Foundation for Research and Innovation. He has been elected in the Deanship of the School of Chemical Engineering of NTUA since 2017. He is one of the founding (in 2014) and organizational members of EMCC and recently joined (in 2020) the OMB of EMMC. From 2010 to 2016 he has been Director of Section III: Materials Science & Engineering of the School, while from 2011 he is Director of the Interdisciplinary Postgraduate (MSc) Program: Materials Science & Technology (NTUA). He has more than 25 years of experience in the fields of Materials Science & Nanotechnology, Carbon-based materials and Safety impacts of Nanotechnology. He has extensive R&D experience through collaborations with international research centers since he has participated in more than 60 European and National funded projects, in many of



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them as Scientific Coordinator (most recent are: Nanotechnologies, Advanced Materials, Advanced Manufacturing and Processing, Resource Efficient Economy with a Sustainable Supply of Raw Materials NMP FP7, Horizon 2020). He is a referee in International scientific journals, evaluator & scientific advisor of R&D projects. He is the author of several scientific books, chapters in international text books and more than 400 scientific publications in peer reviewed international journals and conference proceedings and cited ~6700 by other researchers (h-index 42).

