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Editorial

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Computational materials science is a rapidly developing discipline. As the computational power of computing facilities increases, software packages mature, and data are acquired at higher rates and volumes, the abilities for predicting properties and structure of materials during production or in service continuously progresses. Simulation methods range from the atomic scale of angstroms to the macroscopic scale of industrial plants. While a complete multiscale treatment of materials in silico with a seamless connection of all scales still remains a challenge, a highly integrated approach combining experiments, physics based simulations, and data-driven simulations holds the greatest premises to induce disruptive discovery in materials design and future improvements in materials processing.

The materials modeling community is becoming increasingly connected through large-scale initiatives such as the European Materials Modeling Council (<https://emmc.eu>). The aim is to standardize and bundle materials simulation capabilities and establish a hub for simulation software developers, database creators, materials data provider, software users in industry, and others. Such activities will increase the visibility of computational materials engineering and help bringing materials simulation closer to end-users for whom it is often not straightforward to judge what methods are available and for which purpose they can be applied.

In the following articles, selected topics of computational materials and process engineering are presented to illustrate the current capabilities and methodologies in different Austrian research institutions. The presented simulations address topics which are also of interest for applied research and development in an industrial context.

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