Editorial

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Biographical notes: Timon Rabczuk received his PhD at the University of Karlsruhe. After being a postdoc at Northwestern University (Illinois, USA), Technical University of Munich and a Senior Lecturer at University of Canterbury in New Zealand, he is currently a Full Professor at Bauhaus University Weimar.

Xiaoying Zhuang's key research area is computational materials design for nano composites, metamaterials and nanostructures as well as computational methods for multiphysics and multiscale modelling. He obtained her PhD in Durham University, UK in 2011, which is followed by her Postdoc in Norwegian University of Technology in Trondheim and then as a Faculty Staff in Tongji University. In 2015, she was awarded with the Sofja Kovalevskaja Programme from Alexander von Humboldt Foundation that brought her to Germany and she focused on the modelling and optimisation of polymeric nanocomposite. In 2018, she was awarded with Heinz-Maier-Leibnitz Prize from DFG (German Research Foundation).

The development of new materials, devices and systems has been the research focus in engineering and materials science for many decades. The great value of computational (multiscale) methods to support the design of new materials, devices and systems has been recognised in academia, as well as in the industry. Ford Motors, for example, has put a lot of effort in building a virtual testing laboratory in order to support the manufacturing of power train systems. One key pillar for the design of new materials and structure is modelling and simulation, which helps to come to designs more systematically and faster. Besides such a drastic acceleration, they also reduce associated costs.

The design of new innovative devices and systems involves the optimisation of the system's topology as well as the optimisation of the materials used for the system. For example, the macroscopic properties of a material are the main criteria for its choice for a

particular device. However, the origins of macroscopic material properties reside in the properties and interactions taking place on finer scales. For the design of new materials, it is therefore essential to understand and quantify the links between phenomena on the fine scales and their macroscopic effects. As (experimental) manufacturing and testing is time-consuming, expensive and sometimes unfeasible, computational (multiscale) methods are needed.

This special issue includes several manuscripts about modern numerical methods to advance the field of computational materials design. The contributions in this special issue include not only novel methods such as machine learning-based solutions of partial differential equations, that avoid entirely a classical discretisation and are a natural framework for optimisation and uncertainty analysis, but also interesting applications and advancements in other areas such as optimisation. Challenging topics of this SI are focused on various materials including the impact wear of diesel engines or reinforced concrete. Very valuable is also a comprehensive review paper about the non-local operator method (NOM), a novel theory and computational approach, that also does not require shape functions – similar to the machine learning approach to the solutions of partial differential equations. And finally, the SI is complemented by an interesting contribution about sensitivity analysis that is of high importance in the area of computational materials design.