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Editorial: New Frontiers in Multiscale Modelling of Advanced Materials

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Computer simulations, based on *ab initio*, semi-empirical, or continuum approaches, are now a widespread tool for benchmarking experimental measurements in many areas of engineering, physics, chemistry, and, more recently, biology. Indeed, improved algorithms and increased computational power have widened the areas of application of these computational methods to materials of technological interest, allowing unprecedented access to the investigation of their electronic, optical, thermodynamical, and mechanical properties.

This "third way" represented by the computational lab lies in between the use of pure theoretical models and experiments, and it can be particularly useful when experimental data are difficult to be recorded and theoretical models are too complex to be formulated. In this regard, these methods have been successfully used to investigate and predict properties of matter, ranging from the nanoscale behavior of crystalline materials to their interaction with external fields, e.g., electromagnetic and elastic, and to their macroscopic behavior.

However, they have been commonly adopted via a "single-scale" approach, in which one uses one specific method at each relevant scale. Indeed, this is the simplest approach to face the unfavorable scaling with system size and to beat the time-scale bottleneck. For example, on the one hand, *ab initio* methods, such as density functional theory, have been used to investigate accurately the nanoscale behavior of crystalline materials starting from the first-principles simulation of the electronic motion. On the other hand, coarse-grained methods and discrete mesoscopic models are adopted to assess the properties of materials at atomistic or continuum level. In the latter case, classical molecular dynamics, in connection with fiber bundle or lattice models, numerical and analytical homogenization, and upscaling techniques, as well as finite element or mesh-free approaches, have been successfully used to determine the constitutive laws of materials. Furthermore, the application of these techniques to macroscopic systems enables one to investigate mechanisms, such as fracture, crack, and grain boundary propagation.

Nevertheless, the "single-scale approach" results in a loss of information across different scales and is an important limiting factor in the science of complex materials. A comprehensive vision would allow the exploration of full ranges of materials solutions and hierarchical architectures at all relevant size scales, with the idea that the resulting product is not simply the sum of all the parts. This requires development of new science as well as novel computational methods, since multiscale tools are still in their infancy.

This collection of papers is thus devoted to this rapidly growing field of computational approaches to multiscale methods by reporting a specific set of problems related, but not limited to, materials science. Thus, the reader will find the application and point-of-views on a variety of state-of-the-art

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methods spanning different scales and combining different approaches to bridge the gap between first-principles and continuum-level simulations by matching procedures, both concurrent and hierarchical.

The ambition of this collection is to show how electronic, atomistic, mesoscopic, and continuum models can be combined and integrated to accelerate materials discovery, to shorten the time from "lab-to-market" from the current 10–20 years by avoiding lengthy trial-and-error loops or overlooking other materials not yet discovered for the absence of a multiscale, multiphysics vision.

Crossing the borders between several computational, theoretical, and experimental techniques, this collection should be of interest to a broad community, including experimental and theoretical physicists, chemists, and engineers interested in materials modelling in a broad sense.

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