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Atomistic simulations, based on ab-initio and semi-empirical approaches, are nowadays widespread in many areas of physics, chemistry and, more recently, biology. Improved algorithms and increased computational power widened the areas of application of these computational methods to extended materials of technological interest, in particular allowing unprecedented access to the first-principles investigation of their electronic, optical, thermodynamical and mechanical properties, even where experiments are not available. However, for a big impact on the society, this rapidly growing field of computational approaches to materials science has to face the unfavourable scaling with the system size, and to beat the time-scale bottleneck. Indeed, many phenomena, such as crystal growth or protein folding for example, occur in a space/time scale which is normally out of reach of present simulations. Multi-scale approaches try to combine different scale algorithms along with matching procedures in order to bridge the gap between first-principles and continuum-level simulations. This Research Topic aims at the description of recent advances and applications in these two emerging fields of ab-inito and multi-scale materials modelling for both ground and excited states. A variety of theoretical and computational techniques are included along with the application of these methods to systems at increasing level of complexity, from nano to micro. Crossing the borders between several computational, theoretical and experimental techniques, this Research

Topic aims to be of interest to a broad community, including experimental and theoretical physicists, chemists and engineers interested in materials research in a broad sense.