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Atoms and Computers

Michele Parrinello

Dept. of Chemistry and Applied Biosciences, ETH Zurich,
Istituto di Scienze Computazionali,
Università della Svizzera Italiana, Lugano,
Istituto Italiano di Tecnologia, Genova

Abstract: The rapid development of computer technology and of efficient algorithms has had a deep impact on science. Of particular significance has been the emergence of realistic atomistic simulations. These calculations provide precious insight, replace difficult experiments, predict new phenomena, and are also used to help build the computers of the future that will in turn be used to simulate ever more complex phenomena. We shall illustrate the power of this approach with a number of examples taken from different branches of science. Yet in spite of remarkable progress much remains to be done to widen the scope of atomistic simulations, especially in the fields of nanotechnology and biosciences. This requires new technical as well as conceptual tools in order to describe the complexity of the phenomena that contemporary science has to tackle. Possible avenues of progress will be presented.

