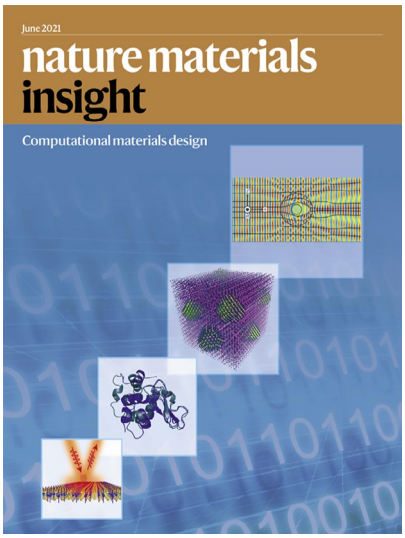

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SPRINGER NATURE LONDON
The Campus, 4 Crinan Street,
London N1 9XW
T: +44 207 833 4000
F: +44 207 843 4563
materials@nature.com

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Computational materials design

The role of computers in scientific research has notably increased over the last several decades. This has been driven by the increasing computational power of these machines as well as more efficient computational approaches, which has enabled the analysis of the increasingly complex materials that are investigated for widely differing needs such as energy, information, or applications at extreme conditions. Better materials need to be designed, but in order to achieve improved materials there needs to be comprehensive insight into behaviour, from the ångström to the micrometre, and from the femtosecond to the millisecond. Computation can certainly help in this endeavour.

In this Insight we aim to capture the role of computation for the understanding, prediction, and design of materials. Different computational methodologies are used to study phenomena at different lengthscales and timescales. Electronic structure methods such as density functional theory can be used to predict the fundamental properties of materials from their smallest constituents: atoms, chemical bonds between atoms, and unit cells, obtaining ground-state properties such as elastic constants as well as excited-state properties such as optical absorption. The study of larger-scale phenomena, for example the bottom-up assembly of nanoparticles into aggregates or crystals, requires less granular but more efficient techniques such as molecular dynamics or Monte Carlo approaches. Multiscale modelling can allow computation to model even greater lengthscales, allowing the determination of properties at sizes directly relevant for engineering, but without sacrificing important information at finer scales. And the rise of machine learning over the last few years has certainly made an impact, allowing the analysis of big data with the extraction of hard-to-see correlations, or the development of improved atomistic approaches that could aid materials design through enhanced accuracy and speedup, and resulting in more reliable descriptions of complex systems.

Many of these approaches are still under active development and refinement. Moreover, the digital infrastructure required to support these simulations, and allow data sharing and validation, is still emerging. The role of computation in providing insight into materials, and enabling materials design, will play a key role in materials innovation. We hope that you enjoy the glimpse into the future of computational materials design that this collection aims to provide. The fast pace of new developments in these research fields will certainly continue to dramatically advance our way of life.

Stephen Shevlin, Senior Editor
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CONTENTS

PERSPECTIVE

Discovering and understanding materials through computation
Steven G. Louie, Yang-Hao Chan, Felipe H. da Jornada, Zhenglu Li and Diana Y. Qiu p728

REVIEW ARTICLES

Electronic-structure methods for materials design
Nicola Marzari, Andrea Ferretti and Chris Wolverton p736

Machine-learned potentials for next-generation matter simulations
Pascal Friederich, Florian Häse, Jonny Proppe and Alán Aspuru-Guzik p750

From predictive modelling to machine learning and reverse engineering of colloidal self-assembly
Marjolein Dijkstra and Erik Luijten p762

Mesoscopic and multiscale modelling in materials
Jacob Fish, Gregory J. Wagner and Sinan Keten p774