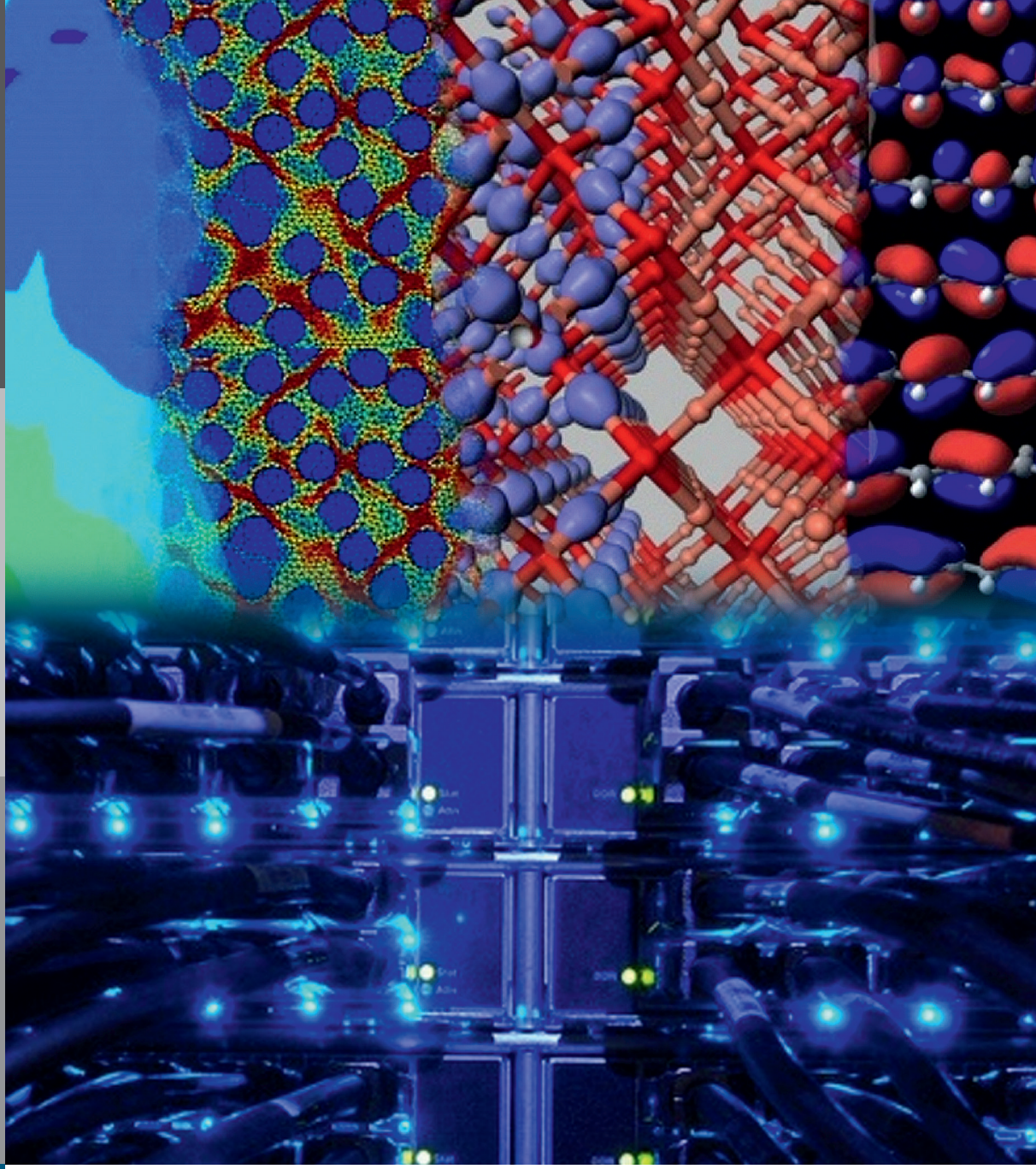

Multiscale Modelling Methods for Applications in Materials Science

Lecture Notes

edited by Ivan Kondov, Godehard Sutmann

cecam
Centre Européen de Calcul Atomique et Moléculaire

JÜLICH
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Forschungszentrum Jülich GmbH
Institute for Advanced Simulation (IAS)
Jülich Supercomputing Centre (JSC)

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CECAM Tutorial, 16 – 20 September 2013
Forschungszentrum Jülich
Lecture Notes

organized by
Karlsruhe Institute of Technology
Forschungszentrum Jülich

Schriften des Forschungszentrums Jülich

IAS Series Volume 19

ISSN 1868-8489 ISBN 978-3-89336-899-0

Contents

Methods

Macroscopic effects in complex materials arise from physical phenomena on multiple length and time scales and therefore properties of such materials can be predicted accurately based on properties of the underlying building blocks. The major benefits of multiscale models are a simpler physical interpretation based on the analysis of sub-models as well as an improved computational scaling making the simulation of very large systems feasible.

This book includes the lecture notes of courses conducted at the CECAM tutorial “Multiscale Modelling Methods for Applications in Materials Science” held at the Jülich Supercomputing Centre from 16 to 20 September 2013. Written by recognized experts the lecture notes complement existing university courses with knowledge and experience gained recently in the field of multiscale materials modelling encompassing theoretical understanding and practical implementation of multiscale models to real-life applications. The book addresses graduate students and young researchers, working in the field of computational materials science, and covers general methodology, tools for implementation of the multiscale modelling paradigm, as well as applications of multiscale modeling techniques. Topics include fields such as coarse graining of polymers and biomolecules, and modelling of organic light-emitting diodes, electrochemical energy storage devices (Li-ion batteries and fuel cells) and energy conversion devices (organic electronics and carbon nanodevices).

This publication was edited at the Jülich Supercomputing Centre (JSC) which is an integral part of the Institute for Advanced Simulation (IAS). The IAS combines the Jülich simulation sciences and the supercomputer facility in one organizational unit. It includes those parts of the scientific institutes at Forschungszentrum Jülich which use simulation on supercomputers as their main research methodology.

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ISBN 978-3-89336-899-0

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