Computational Semiconductor Materials Science

MATERIALS RESEARCH SOCIETY
SYMPOSIUM PROCEEDINGS VOLUME 1370

Computational Semiconductor Materials Science

Symposium held Spring 2011, April 25–29, San Francisco, California, U.S.A.

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MRS
Materials Research Society
Warrendale, Pennsylvania

CAMBRIDGE UNIVERSITY PRESS

CAMBRIDGE UNIVERSITY PRESS
Cambridge, New York, Melbourne, Madrid, Cape Town,
Singapore, São Paulo, Delhi, Mexico City

Cambridge University Press
The Edinburgh Building, Cambridge CB2 8RU, UK

Published in the United States of America by Cambridge University Press, New York

www.cambridge.org
Information on this title: www.cambridge.org/9781605113470

First published 2011

A catalogue record for this publication is available from the British Library

ISBN 978-1-605-11347-0 Hardback

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PREFACE

Recent advances in theory and computational algorithms together with available high-performance computing power have been successfully utilized in the simulation, modeling, optimization, and design of complex materials, especially the semiconductor materials. The progress in computational semiconductor materials sciences has provided significant opportunities to accelerate our understanding of materials properties and guide discovery in semiconductor materials, which will have strong impact in various sciences and technologies and development of new functional devices of technological relevance.

Symposium YY, "Computational Semiconductor Materials Science" held at the April 25–29, 2011 MRS Spring Meeting in San Francisco, California, focused on the theoretical and computational aspects of semiconductor materials and devices. The topics discussed in this symposium cover a broad range from the fundamental theory and computational methods of semiconductor materials to the multi-scale modeling and design of functional semiconductor devices, which include phase change materials, correlated and spintronic materials, photovoltaic and photoelectrochemical materials, spectroscopy of materials, defects in semiconductors, and large scale simulations of alloys, liquids, and amorphous materials. In addition to conventional bulk and thin film semiconductors, electronic and transport properties of carbon nanostructures, transition-metal oxides, and related semiconductor nanostructures are also included.

The symposium was well attended with a strong international participation. Works presented in this symposium were given as invited talks, oral talks, and posters, which reflect very well the state of the art in the computational semiconductor materials science. The symposium confirms the vital roles of computational semiconductor sciences played in modern scientific research. This proceedings volume contains eighteen peer-review papers, which provide the readers with valuable insights into their respective research fields. We hope that it will be a useful reference source for researchers in these fields.

We wish to thank all of the participants including an outstanding roster of invited speakers, session chairs, and MRS staff for making the symposium a successful event. We would like to express our sincere thanks to the authors and reviewers of the papers in this proceedings volume for their timely submission and review of the papers.

Su-Huai Wei
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August 2011

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