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Preface

These conference proceedings contain the written papers of the contributions presented at the 4th International Conference on Theory, Modelling and Computational Methods for Semiconductor materials and nanostructures. The conference was held at the MediaCityUK, University of Salford, Manchester, UK on 22–24 January 2014. The previous conferences in this series took place in 2012 at the University of Leeds, in 2010 at St William’s College, York and in 2008 at the University of Manchester, UK.

The development of high-performance computer architectures is finally allowing the routine use of accurate methods for calculating the structural, thermodynamic, vibrational, optical and electronic properties of semiconductors and their hetero- and nano-structures. The scope of this conference embraces modelling, theory and the use of sophisticated computational tools in semiconductor science and technology, where there is substantial potential for time-saving in R&D. Theoretical approaches represented in this meeting included: Density Functional Theory, Semi-empirical Electronic Structure Methods, Multi-scale Approaches, Modelling of PV devices, Electron Transport, and Graphene. Topics included, but were not limited to: Optical Properties of Quantum Nanostructures including Colloids and Nanotubes, Plasmonics, Magnetic Semiconductors, Photonic Structures, and Electronic Devices. This workshop ran for three days, with the objective of bringing together UK and international leading experts in the theoretical modelling of Group IV, III-V and II-VI semiconductors, as well as students, postdocs and early-career researchers. The first day focused on providing an introduction and overview of this vast field, aimed particularly at students, with several lectures given by recognized experts in various theoretical approaches. The following two days showcased some of the best theoretical research carried out in the UK in this field, with several contributions also from representatives of renowned theoretical groups from many European countries (Spain, France, Ireland, Germany, Switzerland, Luxemburg, Norway, Italy, Poland, Denmark, Sweden, Serbia, etc.), as well as Asia (Iran, Japan) and USA.

We would like to thank all participants for making this a very successful meeting and for their contribution to the conference programme and these proceedings. We would also like to acknowledge the financial support from the Institute of Physics (Semiconductor Physics Group and Computational Physics Group), EPSRC-UK, the CECAM UK-Hartree Node, CCP9, and Quantum Wise (distributors of Atomistix).

The Editors



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The proceedings were edited and compiled by Joydeep Pal, Max Migliorato and Stanko Tomić.