PREFACE

Selected contributions from the 3rd Theory Meets Industry International Workshop, TMI2009 (Nagoya, Japan, 11–13 November 2009)

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PREFACE

Selected contributions from the 3rd Theory Meets Industry International Workshop, TMI2009 (Nagoya, Japan, 11–13 November 2009)

Guest Editors

Isao Tanaka
Kyoto University and Japan Fine Ceramics Center, Japan

Jürgen Hafner
University of Vienna, Austria

Erich Wimmer
Materials Design Inc., USA

Ryoji Asahi
Toyota Central R&D Labs, Japan

The structures, physicochemical and thermodynamic properties of materials are becoming increasingly amenable to treatment by first-principles (ab initio) quantum mechanical simulations. Calculations containing a few hundred atoms are now routine, thanks to improvements in computer technology and computational techniques. Schemes to determine electronic structures more accurately and to treat more complex systems continue to be developed. A growing number of scientists and engineers are becoming aware of the power of these approaches. By applying these new computational tools, materials science and technology is expected to enter a new era of accelerated progress and efficiency.

In 1998 the first workshop entitled ‘Theory Meets Industry’ (TMI) was held at the Vienna University of Technology. The aim of the workshop was to direct the potential of the ab initio simulation codes developed in academia towards the necessities arising from industrial research. Over the next decade, significant advances in ab initio methodology and its application to academic and industrial research were achieved. It was thus considered timely to hold a second TMI workshop in 2007, again in Vienna. The contributions from academia concentrated on a wide range of new developments in ab initio simulations, as well as on applications at the forefront of materials research. Speakers from the industrial sector also emphasized the progress made in successfully applying ab initio techniques to key areas of modern technology. The proceedings were published in Journal of Physics: Condensed Matter as a special issue (volume 20, number 6, 2008), which was included in the ‘Top papers 2008 showcase’ of that journal.

Following the notable success of the first two workshops, it was decided that the third TMI workshop would be held outside Europe. Holding the workshop in Japan was intended to increase awareness of theoretical materials science and foster further international collaboration in this field. Lectures and poster presentations were thus solicited from leading international academic and industrial researchers. The large audience that attended responded to the high quality of the talks with pertinent questions and lively discussions.

The third workshop, TMI2009, was held over three days from 11–13 November, 2009, at the Nagoya International Center, Nagoya, Japan. Invited talks were given by 23 speakers from 9 countries from both the academic and industry sectors. The speakers were Ryoji Asahi (Toyota Central R&D Labs, Japan), Tomas Bucko (University of Vienna, Austria), Gábor Csányi (University of Cambridge, UK), Alessandro De Vita (King’s College London, UK), Bernard Delley (Paul Scherrer Institute, Switzerland), Christophe Domain (EDF, France), George Fitzgerald (Accelrys, USA), Takeo Fujiwara (University of Tokyo, Japan),
Jürgen Hafner (University of Vienna, Austria), Masaya Ishida (Sumitomo Chemicals, Japan), Werner Janse Van Rensburg (Sasol Technology, South Africa), Masanori Kohyama (AIST, Japan), Takao Kotani (Tottori University, Japan), Georg Kresse (University of Vienna, Austria), Katsuyuki Matsunaga (Kyoto University, Japan), Stefan Müller (University of Erlangen-Nuremberg, Germany), Shin-ichiro Nakamura (Mitsubishi Chemicals, Japan), Fumiyasu Oba (Kyoto University, Japan), Tamio Oguchi (Hiroshima University, Japan), Pascal Raybaud (IFP, France), Isao Tanaka (Kyoto University/JFCC, Japan), Göran Wahnström (Chalmers University of Technology, Sweden), and Erich Wimmer (Materials Design Inc., USA). There were 40 poster presentations in total. The workshop was attended by approximately 120 participants with approximately 50 per cent from industry.

The invited talks covered advances in ab initio solid-state calculations and their practical use in industry. Presentations outlining the progress made in treating large and complex systems, as well as more accurate and efficient calculation methods, were given from the theory side. Examples of the use of ab initio calculations for research and development of a wide variety of materials were presented from the application side. These included materials for fuel cells, solar cells, lithium batteries, heterogeneous catalysts, oxide semiconductors, bioceramics, light-emitting devices, and many others. It is clear that the gap between theory and application is becoming ever narrower, and collaboration between industry and academia is now de rigueur. Some researchers in industry use ab initio tools every day as part of their research and development activities. The language gap between industry and theory is also narrowing, as shown by the active discussions between presenters and audience.

TMI2009 was a satellite meeting of the 2nd International Symposium on Advanced Microscopy and Theoretical Calculations (AMTC2), held from 24–26 June, 2010, in Nagoya, Japan. The AMTC series of meetings was organized to commemorate the establishment of the Nanostructures Research Laboratory (NSRL) at the Japan Fine Ceramics Center (JFCC), and as a daughter event of EXPO 2005 Aichi, Japan. We would like to express our thanks to all the staff of the NSRL who helped run the workshop and contributed immeasurably to its success. Financial support for the workshop from the Grant-in-Aid for Scientific Research on Priority Areas ‘Nano Materials Science for Atomic-Scale Modification’ from the Ministry of Education, Culture, Sports and Technology (MEXT) and Psi-k Network is also gratefully acknowledged.

All submitted papers in this special issue were reviewed in order to meet the high standards of Journal of Physics: Condensed Matter. We are grateful to the many anonymous referees who made this possible. Last but not least, we would also like to thank all invited and poster contributors (especially those who accepted the burden of writing a full paper), and the Institute of Physics for their help in the preparation of this special issue.