

Proceedings of the Second Workshop on Theory meets Industry (Erwin-Schrödinger-Institute (ESI), Vienna, Austria, 12–14 June 2007)

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**FOREWORD**

# Proceedings of the Second Workshop on Theory meets Industry (Erwin-Schrödinger-Institute (ESI), Vienna, Austria, 12–14 June 2007)

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The development of modern materials science has led to a growing need to understand the phenomena determining the properties of materials on an atomistic level. As the behavior of atoms and electrons is governed by the laws of quantum mechanics, accurate and efficient techniques for solving the basic quantum-mechanical equations for very complex many-atom, many-electron systems are required. The development of density-functional theory (DFT) represents a decisive step forwards in our efforts to develop tools for *ab initio* atomistic simulations of complex materials, preparing the way towards computational materials design.

The development of these *ab initio* simulation methods, whose aim is to model processes in materials by solving the coupled Newtonian equations of motion of the atoms and the Schrödinger equation for the electrons from first principles without any other input than the atomic numbers of the constituents, is part of fundamental research. Hence, for a long time the development and application of DFT methods has been a domain of academic research. Only during the past decade, based on the development of increasingly sophisticated codes and better computer performance, has the impact of DFT-based simulation methods spread from academia to industry. New opportunities are opening for innovative materials research across physics, chemistry, surface science and nanotechnology extending even to earth sciences and molecular biology.

In 1998 we organized, at the Vienna University of Technology, a first workshop entitled ‘Electronic Structure Calculations for Industry and Basic Sciences’ (short title ‘Theory meets Industry’) to celebrate the start of the European Science Foundation (ESF) research program ‘Electronic Structure Calculations for Elucidating the Complex Atomistic Behavior of Solids and Surfaces’, known as the  $\Psi_k$ -network. At this workshop, researchers from academia presented recent results in the development of *ab initio* simulation methods and their application to key areas of condensed matter physics. Researchers from industry mainly focused on challenges arising from applied industrial research; contributions describing successful applications of DFT techniques to industrial problems were more scarce.

Progress during the last decade has been very fast. The ESF research program has been renewed under the much bolder title ‘Towards Computational Materials Design’ and is now approaching the end of this second funding period. Due to the development of accurate, efficient and stable software packages for *ab initio* simulations, DFT-based techniques are now routinely used in many industrial laboratories worldwide. It was therefore considered timely to organize a second ‘Theory meets Industry’ workshop.

The meeting took place between 12–14 June 2007 at the Erwin-Schrödinger-Institute (ESI) for Mathematical Physics in Vienna (Austria). It was sponsored by the Universität Wien through the VASP (Vienna *Ab-Initio* Simulation Program) project, the Center for Computational Materials Science Vienna, the Erwin-Schrödinger-Institute and the ESF Program ‘Towards Computational Materials Design’. The program of the workshop was decided by an international advisory board consisting of Ryoji Asahi (Toyota Central Research and Development Laboratory), Risto Nieminen (Helsinki University of Technology), Herve Toulhoat (Institut Français du Pétrole), Erich Wimmer (Materials Design Inc.), Chris Wolverton (Ford Motor Co. and Northwestern University) and Jürgen Hafner (Universität Wien). The 35 invited talks presented at the meeting were divided equally between researchers from academia and from industry. The contributions from academia concentrated on a wide range of new developments in DFT and post-DFT simulations (with contributions from the developers of leading software packages for *ab initio* simulations), as well as on applications in front-line materials research. In contrast to the first workshop nine years ago, all industrial speakers presented results of extensive *ab initio* studies in key areas of modern technology, concentrating on catalysis and chemical processing, information technologies, automotive engineering and energy.

The proceedings assemble full papers summarizing 23 of the invited talks, abstracts of the remaining invited talks and abstracts of all the poster contributions. It is complemented by a conference summary written by Erich Wimmer. Erich is certainly excellently qualified for this task, because for many years he has played the role of mediator between academia and industry. I shall not anticipate his summary here, but I think that it is fair to say that tremendous progress has been made since the first workshop. *Ab initio* DFT simulations are now a well established tool for industrial research and, due to the availability of cheap high-performance server clusters, their use is no longer the reserve of large corporate laboratories equipped with supercomputers, but are also accessible to medium-sized enterprises. The basic methodology is still developed by the leading academic research groups. These groups urgently need support from funding agencies and/or industry not only for the basic code development, but also to bring their research codes up to industrial standards of programming, stability, user-friendliness and documentation.

The fundamental challenge to theory, however, remains the same: more accurate total energies, application to larger and even more complex systems, and access to new materials properties. Responding to these challenges will require substantial effort at various levels. Achieving greatly improved accuracy of calculated total energies demands an improved description of electronic exchange and correlation. Possible routes (hybrid functionals for solids, dynamical mean field theory (DMFT), many-body perturbation theory (GW), quantum Monte-Carlo) have been presented at this meeting. Access to larger systems could be realized either by codes achieving  $O(N)$ -scaling or by adopting a strategy of multi-scale simulations. At least two different  $O(N)$ -codes have been discussed at the workshop. But even if these approaches allow *ab initio* calculations to be performed for ten times as many atoms as before, in terms of linear dimensions, the accessible systems size increases only by a factor of two. Therefore, multi-scale simulations strategies remain a very important issue. Access to new materials properties requires adding new routines to the basic codes. Again, this meeting has highlighted important new developments: evolutionary crystal structure predictions, transport properties of semiconductors and insulators, and calculations of free-energy reaction barriers to name only a few.

The task of providing a full ‘tool-box’ of routines for fast and efficient calculation of many different materials properties evidently exceeds the capacity of a single group of developers. Here, collaboration is necessary between the developers of the basic DFT codes and the expert users of these codes pushing the application of the methodology to new frontiers. Again, it will be important to bring the newly developed routines into a stable, well documented form and to make them accessible to a wide range of users, both in academia and industry. Supporting these efforts is also a challenge to industry. The academic research needs industry’s support in many ways. Industry has to make governmental and funding agencies aware of the vital role of our research for future technological development—and a very persuasive way to do that is to invest directly into leading academic groups.

As the workshop organizer and editor of the proceedings, I would like to thank all contributors (especially those who accepted the burden of writing a full paper), the members of the Advisory Board for helping to organize such a good program, and the Institute of Physics for their help in the preparation of the proceedings.