



## WORKSHOP

# ”THEORY MEETS INDUSTRY” THE IMPACT OF DENSITY-FUNCTIONAL CALCULATIONS ON MATERIALS SCIENCE

JUNE 12-14, 2007

ERWIN-SCHRÖDINGER-INSTITUTE FOR MATHEMATICAL  
PHYSICS

Boltzmannngasse, A-1090 WIEN, AUSTRIA

sponsored by

**Center for Computational Materials Science, Wien**  
**Erwin Schrödinger Institute for Mathematical Physics, Wien**  
**Universität Wien**  
**ESF Research Programme ”Towards Computational Materials Design”**

### Scientific Scope

In 1998 a workshop called ”Theory Meets Industry” was held at the Technical University in Wien to celebrate the start of the Research Programme ”Electronic Structure Calculations for Elucidating the Complex Atomistic Behavior of Solids and Surfaces” sponsored by the European Research Foundation (ESF) - better known as the ”psik-network”. The aim of the workshop was to confront the potential of the ab-initio simulation codes developed in academia with the necessities arising from industrial research.

The Research Programme has been renewed under the title ”Towards Atomistic Materials Design” and is now approaching the end of the second funding period. Everybody will agree that much progress has been realized since the 1998 workshop and that density-functional theory develops an increasingly important impact on materials research, not only in academia, but also in industry. Therefore it was timely to organize a second workshop ”Theory Meets Industry”. The workshop took place on June 12-14 in the Erwin-Schrödinger Institute in Wien. The scientific program was planned by a Scientific Advisory Board (SAB) consisting of Risto Nieminen (TU Helsinki), Chris Wolverton (Ford Motors and NWU Evanston), Herve Toulhoat (Institut Francais du Petrole), Ryoji Asahi (Toyota), Erich Wimmer (Materials Design) and Jürgen Hafner (U Wien).

As for the previous meeting the aim was to highlight the most recent progress in the development of ab-initio density-functional, post-DFT methods and in front-line applications in academia and to present recent achievements in industrial research. About 40 talks and posters, coming in an equal percentage from researchers in academia and industry, have been presented. the full program of the meeting and abstracts of all contributions are appended. Proceedings of the workshop will be published in a special issue of the Journal of Physics: Condensed Matter.