INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

Monday, 7 November, 4:00 p.m.
Room IC 02-718

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Computational Materials Research in an Industrial Context

We are currently witnessing an increasingly important role of computational materials research in industry. Three main factors are enabling this development, (i) the remarkable progress in computational methods, (ii) the availability of enormous computing power, and (iii) the development of sophisticated software environments for materials modelling. Together, these capabilities are providing unprecedented opportunities for industrial research. This lecture will illustrate the deployment of these computational approaches in solving problems in “green electronics”, irradiation effects in Zr alloys, Li-ion batteries, polymers, and CO_2 capture. These examples demonstrate that computational materials research is thus making increasingly valuable contributions to sustainable and environmentally responsible technologies.

Biosketch of Erich Wimmer

Erich Wimmer is co-founder and Chief Scientific Officer of Materials Design, a company developing software and providing services for materials research. He received an engineering degree in 1974 from the University of Technology in Vienna and a doctoral degree in chemistry in 1977 from the same institution. As research associate with Prof. A. J. Freeman at Northwestern University, Illinois, USA, Dr. Wimmer was instrumental in the development of the highly accurate FLAPW method for calculating structural and electronic properties of solids and surfaces. In 1985 he joined Cray Research in Minnesota as Technical Director, where he initiated and headed an industrial consortium to develop a new generation of software for materials modeling ("UniChem"). In 1992 he was hiredby Biosym Technologies in San Diego to start an industrial consortium in electronic, optical, and magnetic materials. During the past two decades at the company Materials Design he has been leading

a team focusing on the prediction of materials properties and mechanisms such as hydrogen pickup in zirconium alloys using advanced first-principles quantum mechanical approaches in combination with atomistic molecular dynamics and Monte Carlo simulations. Dr. Wimmer is author and co-author of over 130 scientific publications and book contributions. He has given numerous invited talks worldwide. Dr. Wimmer has been selected as “Outstanding Referee” by the American Physical Society. He served on the scientific advisory board of the Thomas Young Centre, the London Centre for Theory and Simulation of Materials in the U.K. and he is chairman of the industrial advisory board of the MARVEL project at the Ecole Polytechnique Fédérale de Lausanne in Switzerland.