

***Ab initio* design of structural materials**

FEBRUARY 14-15, 2003
Ångströmlaboratoriet, Uppsala, Sweden

PRELIMINARY PROGRAMME

Antonis N. Andriotis (Greece),

Nanotubes and Nanoclusters : Ab initio and semi-empirical studies

Michele Catti (Italy),

Piezoelectric and ferroelectric properties of crystals by ab initio periodic LCAO calculations

H. Dreysse (France),

Title to be announced

H. Ebert (Germany),

The Munich SPR-KKR program package -recent developments and future extensions

Olle Eriksson (Sweden),

Transition metal carbides, from theory to technology

Adam Kiejna (Poland),

Adsorbate structures on metal and oxide surfaces

Janos Kollar (Hungary),

Title to be announced

A. Lichtenstein (The Netherlands),

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Juan J. Novoa (Spain),

Theoretical studies of purely organic molecular magnets

Nicolas Papanicolaou (Greece),

Semi-empirical interatomic potentials from first-principles total-energy calculations

Krzysztof Parlinski (Poland),

Phonons dispersion curves, soft modes, and phase transitions.

Olivier Le Bacq (France), Alain Pasturel (France), and O. Bengone (Sweden),

Optimized lithium orthophosphates for battery cathodes

Anthony T. Paxton (UK),

'Zirconia'

Hariton Polatoglou (Greece),

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A. V. Ruban (Denmark),

Configurational thermodynamics of metallic alloys from first-principles

S. I. Simak (Sweden),

Ordering in multicomponent alloys from first principles

Thomas Bligaard (Denmark),

Combined DFT and Evolutionary Search for Materials Design

V. S. Stepanyuk (Germany)

Magnetism, Structure and Interactions on the atomic scale

I. Turek (Czech Republic),

Magnetovolume effect in RECo₂ intermetallics

Levente Vitos (Hungary),

EMTO-CPA method: an implementation and selected applications

Perla Wahnón (Spain),

Novel Intermediate Band Materials for High Efficiency Solar Cells Designed by First Principles

Rudolf Zeller (Germany),

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Yu.Kh.Vekilov (Russia),

"Quasicrystals and their applications"