

## Recent additions to the links on the CCP5 WWW pages

M. Leslie

The CCP5 WWW pages have a page which contains a list of links to the research pages of other members of CCP5. Links are added to this list when new members register, or when a speaker is invited to give a talk at one of CCP5's meetings. Relevant links will also be added on request to the CCP5 secretary at the above address. The URL for the page is <http://www.dl.ac.uk/CCP/CCP5/links.html> I have given below a list of links I have added recently together with a line indicating the nature of the research. I have not included the URL's of the pages as these may be more easily found from the CCP5 Web page given above.

Professor David Srolovitz    Department of Materials Science and Engineering  
University of Michigan

Research studies center on defects in crystals and the formation and evolution of microstructure and morphology.

Roger Smith                    Department of Mathematical Sciences  
Loughborough University

Materials modelling, particularly of semi-conductor processing and nanotechnology; fullerenes; continuum and cellular models of surface propagation; particle ejection from ion-bombarded surfaces; modelling weld phenomena; molecular Dynamics simulations of metals, polymers and covalent materials; global optimisation of molecular structures.

Tuck Choy                    Department of Physics  
Monash University

Research Areas: Theoretical Condensed Matter Physics Worked on Superconductivity, Statistical Mechanics, Hubbard Models, Semiconductors, Porous Silicon, STM, Many - Body Theory, Positron Annihilation and Microwave Absorption.

Condensed Matter The-    Institute of Physics  
ory Group                    Johannes Gutenberg-University Mainz

Statistical thermodynamics of solids and liquids. Starting from atomistic descriptions, cooperative phenomena in thermal equilibrium are investigated, for instance phase transitions and critical phenomena. But also phenomena and/or processes out of equilibrium are studied.

Dr. Peter Gumbsch            Max-Planck Institut fur Metallforschung,  
D-70174 Stuttgart, Germany.

Dislocations Faster than the Speed of Sound; Application of DDD to thin film plasticity; Finite Element - Atomistic Coupling; Lattice Trapping of Fracture Cracks; Directional Anisotropy in Cleavage Fracture ; MD Simulation of Dynamic Fracture Processes; Debye-Waller Factors of NiAl.

Professor A.D.MacKerell    Department of Pharmaceutical Science,  
University of Maryland,

Active areas of research include the development of parameters for empirical force field calculations of molecules of biological and pharmaceutical interest and the application of theoretical approaches towards the elucidation of biochemical mechanisms and the rational design of drugs.

Dr J A Anwar                      Department of Pharmacy  
King's College London

Computer simulation of molecular systems; Crystallisation and crystal engineering; Polymorphism and polymorphic phase transformations; Solid state chemistry; X-ray and Neutron diffraction.

Prof. Paul Madden              Physical and Theoretical Chemistry Laboratory,  
University of Oxford

Recent publications include

“Covalent” effects in “ionic” systems. *Chem. Soc. Reviews* 25, 339 (1997)

Polarization effects, network dynamics and the infrared spectrum of amorphous SiO<sub>2</sub> *Phys. Rev. Letters* 77, 4023 (1996).

Cluster formation in sodium-doped zeolite-Y. *J. Phys. Chem.* 99, 6697 (1995).

Peter Ahlström                    Materials and surface physics group,  
Applied Physics,  
School of Physics and Engineering Physics  
Chalmers University of Technology and Göteborg University.

Computer simulations at the border between physics and chemistry, especially concerning phenomena at surfaces and interfaces. Calculation of vibrational spectra and other properties of oligomers and polymers of propylene oxide via MD simulations. Modelling of water (ice) adsorbates on platinum. Studies on pressure calculation in molecular simulations.

Grant D. Smith                    Department of Materials Science & Engineering  
University of Utah  
Department of Chemical & Fuels Engineering  
University of Utah

Research in the group is concerned with elucidating property/structure relationships in soft condensed matter, with particular emphasis on polymer structure and dynamics. Modeling and experimental methods are used to study static and dynamic properties of polymer melts and glasses, polymer interfaces, and polymers in aqueous solution.

Carol K. Hall                      Department of Chemical Engineering  
North Carolina State University.

Areas of interest: Molecular thermodynamics and computer simulation, equations of state, polymer



