
Contents

Physics

<i>H. Ruder and R. Speith</i>	1
Chain Conformations and Phase Behavior in Confined Polymer Blends <i>A. Cavallo, M. Müller and K. Binder</i>	3
Thermal Quark Anti-quark Free Energies, Energies and Screening in Hot SU(3) Gauge Theory <i>O. Kaczmarek, F. Karsch, P. Petreczky, and F. Zantow</i>	17
Simulations of Particle Suspensions at the Institut für Computerphysik <i>A. Komnik, M. Strauß, S. McNamara, and H. Herrmann</i>	27
Numerical Modelling of Convection and Dynamo Processes in Fully Convective Stars <i>W. Dobler</i>	39
Large Scale Simulation of a Cooled, Pulsed Jet in Symbiotic Stars <i>M. Stute and M. Camenzind</i>	47
Image States on the LiF(001)-(1×1) Insulator Surface <i>M. Rohlfing</i>	57
Interaction of Jets with Galactic Winds <i>M. Krause and M. Camenzind</i>	67
Solid State Physics	
<i>W. Hanke</i>	79
Numerical Studies of Model Colloids and Nano-Wires <i>M. Dreher, K. Franzrahe, P. Henseler, W. Strepp, and P. Nielaba</i>	83
Ab Initio Simulation of Clusters: Relativistic Effects in Structure and Bonding of Noble Metal Nanoparticles <i>M. Moseler, H. Häkkinen, and B. v. Issendorff</i>	95

The Mixed Alkali Effect in Ternary Alkali Silicate Melts: Insight from Molecular Dynamics Computer simulations <i>H. Knoth, J. Horbach, and K. Binder</i>	107
Methylchloride Adsorption on Si(001) – Electronic Properties <i>M. Preuß, W.G. Schmidt, and F. Bechstedt</i>	115
Dynamics and Criticality of Correlated Electrons and Quantum Gases <i>C. Lavallo, M. Rigol, J. Hub, and A. Muramatsu</i>	129
Electron-doping Evolution of the Quasiparticle Band of the Cuprates <i>C. Dahnken, M. Potthoff, E. Arrigoni, and W. Hanke</i>	141
Computational Fluid Dynamics	
<i>S. Wagner</i>	153
Investigation of Hypersonic Flat-plate Boundary-layer Transition by Direct Numerical Simulation <i>C. Stemmer and N.A. Adams</i>	155
DNS Study of spatial discrete suction for Laminar Flow Control <i>R. Messing and M. Kloker</i>	163
LES of Shock Wave/Turbulent Boundary Layer Interaction <i>M.S. Loginov, N.A. Adams, and A.A. Zheltovodov</i>	177
Large-eddy Simulation of Incompressible Flow Around a Sphere with Trip Wire at Re=50 000 <i>M. Torlak, G. Jensen, and I. Hadžić</i>	189
LES of Passive Heat Transfer in a Turbine Cascade <i>J.G. Wissink and W. Rodi</i>	201
Enhanced Mixing in Supersonic Combustion <i>F. Schneider, P. Gerlinger, and M. Aigner</i>	213
Numerical Study of the Influence of Dynamic Pressure and Deflected Ailerons on the Deformation of a High Speed Wing Model <i>C. Braun, A. Boucke, and J. Ballmann</i>	225
Numerical High Lift Research II/III <i>S. Melber-Wilkending, A. Stürmer, E. Stumpf, J. Wild, and R. Rudnik</i>	237
Numerical Simulation of Electrostatic Spray-painting Processes in the Automotive Industry <i>Q. Ye, J. Domnick, A. Scheibe, and K. Pulli</i>	261

Combination of Detailed CFD Simulations Using the Lattice Boltzmann Method and Experimental Measurements Using the NMR/MRI Technique <i>T. Zeiser</i>	277
Recent Improvements of the Parallel-Multiblock URANUS 3D Nonequilibrium Code <i>M. Fertig, F. Infed, F. Olawsky, M. Auweter-Kurtz, and P. Adamidis</i> ...	293
Chemistry	
<i>C. van Wüllen</i>	311
The Iron(III) Catalyzed Michael Reaction – Reactivity Differences Between Several Different Acceptors <i>S. Pelzer and C. van Wüllen</i>	315
Potential Energy Surfaces of Unusual Double Proton Transfer Reactions <i>G. Rauhut and S. Schweiger</i>	323
Quantum Reactive Scattering for Ion-neutral Collisions: The H_3^- -system <i>C. Morari and R. Jaquet</i>	333
Glycine at the Water / Pyrite Interface Under Extreme Pressure / Temperature conditions <i>C. Boehme, E. Schreiner, and D. Marx</i>	349
Computer Science	
<i>C. Zenger</i>	357
Performance Analysis of NEC Computers by Using the PARbench Benchmark System <i>A. Kowarz, W.E. Nagel, and B. Trenkler</i>	359
SKaMPI – Towards Version 5 <i>W. Augustin, M. Haller, M.-O. Straub, and Th. Worsch</i>	371
Earth Sciences	
<i>E. Krause</i>	383
Numerical Considerations of Fluid Effects on Wave Propagation <i>E.H. Saenger, O.S. Krüger, and S.A. Shapiro</i>	385
Toward a Thermochemical Model of the Evolution of the Earth's Mantle <i>U. Walzer, R. Hendel, and J. Baumgardner</i>	395