Appendix A

Schedule of the 1994 GICC School of Computational Chemistry

19 September

Morning Session

8.30	-	10.30	D. Viterbo:	The Language of Space Group Theory
11	-	12	R. Dovesi:	The Language of Band Theory
12	-	13	C. Roetti:	The HF-LCAO (CRYSTAL) Technique

Afternoon Session.
Use of the International Tables of Crystallography (Viterbo, Ugliengo, Aprà)
Graphical tools for periodic Systems (Harrison)

20 September

Morning Session

8.30	-	10.30	C. Pisani:	Ab-initio Quantum-Mechanical Treatment of Periodic Structures
11	-	12	K. Schwarz:	The DF-LAPW Technique
12	-	13	A. Dalcorso:	The PW-SCF Technique

Afternoon Session.
Guide to the use of the PWSCF and CRYSTAL programs (Dalcorso, Roetti, Orlando, Aprà)

21 September

Morning Session

8.30	-	9.30	V.R. Saunders:	The Coulomb Problem in Periodic Structures; Ewald Technique
9.30	-	10.30	R. Dovesi:	Crystal Energy, Elastic Properties, Phase Transitions
11	-	13	M. Catti:	Lattice Dynamics and Thermodynamic Properties

Afternoon Session.
Choice of Basis Set and Use of Pseudopotentials (Roetti, Dalcorso, Orlando, Aprà)
Estimate of Formation Energies and of Correlation Corrections (Dalcorso, Orlando, Causà, Aprà)

22 September

Morning Session

8.30	-	9.30	M. Causà:	Numerical Integration in LCAO-DFT Techniques
9.30	-	10.30	A. Dalcorso:	Special Point Techniques for Reciprocal Space Integration
11	-	12	N.M.H. Harrison:	Direct SCF and Parallel Algorithms for Crystalline Systems
12	-	13	E. Aprà:	Magnetic Properties of Crystalline Systems

Afternoon Session.
The Bader Analysis of Crystalline Electron Charge Densities (Gatti)
Magnetic Properties of Crystalline Systems (Dovesi, Aprà)

23 September

Morning Session

8.30	-	10.30	M. Weyrich:	Density matrix; Structure Factors, Compton Profiles
11	-	13	R.Resta:	Induced and Spontaneous Dielectric Polarization

Afternoon Session.
X-Ray Structure Factors and the Problem of the Thermal Corrections (Lichanot, Dovesi, Roetti)
Calculation of Compton Profiles (Asthalter)

24 September

Morning Session

8.30	-	9.30	M. Rasetti:	The Hubbard Model and Superconductivity
9.30	-	10.30	V.R. Saunders:	The Electronic Correlation in Crystals
11	-	12	C. Pisani:	Loss of Symmetry: Surfaces and Local Defects

Appendix B

Subject Index

Appendix C

List of Acronyms

AFM – Antiferromagnetic
AO – Atomic Orbital
APW – Augmented Plane Wave
ASA – Atomic Sphere Approximation
ASW – Augmented Spherical Wave
a.u. – atomic units
BCS – Bardeen, Cooper and Schrieffer
BF – Bloch Function
BHS (PP) – Bachelet, Hamann and Schlüter (Pseudo-Potentials)
BO – Born-Oppenheimer (approximation)
BSSE – Basis Set Superposition Error
BZ – Brillouin Zone (first)
CC – Coupled-Cluster
CFLS – Cluster Fermionic Linearization Scheme
CMO – Canonical Molecular Orbital
CO – Crystalline Orbital
CP – Car-Parrinello
CPU – Central Processing Unit
DF(T) – Density Functional (Theory)
DM – Density Matrix
DOS – Density of States
ECP – Effective Core Potentials
EFG – Electric Field Gradient
FFT – Fast Fourier Transform
FLAPW or FP-LAPW – Full-potential Linearised Augmented Plane Wave
FM – Ferromagnetic
FWHM – Full Width Half Maximum
GC – Gradient-Corrected
GFMC – Green-Function Montecarlo
GGA – Generalised Gradient Approximation
GS(ES) – Ground State (Electronic Structure)
GT(O) – Gaussian Type (Orbital)
KS – Kohn and Sham
HC – Host Crystal
HF – Hartree-Fock
IDOS – Integrated Density of States
IR – Irreducible Representation
KKR – Korringa-Kohn-Rostoker
LAPW – Linearised Augmented Plane Wave
LCAO – Linear Combination of Atomic Orbitals
LDA – Local Density Approximation
LMO – Localised Molecular Orbital
LMTO – Linear Muffin-Tin Orbital
LO – Local Orbital
LSDA – Local Spin Density Approximation
MD – Molecular Dynamics
MIT – Metal-Insulator Transition
MO – Molecular Orbital
MT(A) – Muffin Tin (Approximation)
NSG – Natural Spin Geminal
NSO – Natural Spin Orbital
ODLRO – Off-Diagonal Long-Range Order
PDOS – Projected Density of States
PP – Pseudo-Potential
PW – Plane Wave
QM – Quantum Mechanics
RIM – Rigid Ion Model
ROHF – Restricted Open-shell Hartree-Fock
RHF – Restricted Hartree-Fock
RIF – Residual Instrumental Function
SC – Supercell
SCF – Self-Consistent-Field
SIC – Self-Interaction Correction
SM – Shell Model
STO – Slater Type Orbital
TG – Translation Group
UHF – Unrestricted Hartree-Fock
VMC – Variational Montecarlo

Springer and the environment

At Springer we firmly believe that an international science publisher has a special obligation to the environment, and our corporate policies consistently reflect this conviction.

We also expect our business partners – paper mills, printers, packaging manufacturers, etc. – to commit themselves to using materials and production processes that do not harm the environment. The paper in this book is made from low- or no-chlorine pulp and is acid free, in conformance with international standards for paper permanency.

Springer

Lecture Notes in Chemistry

For information about Vols. 1–29
please contact your bookseller or Springer-Verlag

Vol. 30: R.D. Harcourt, Qualitative Valence-Bond Descriptions of Electron-Rich Molecules: Pauling "3-Electron Bonds" and "Increased-Valence" Theory. X, 260 pages. 1982.

Vol. 31: H. Hartmann, K.-P. Wanczek, Ion Cyclotron Resonance Spectrometry II. XV, 538 pages. 1982.

Vol. 32: H.F. Franzen Second-Order Phase Transitions and the Irreducible Representation of Space Groups. VI, 98 pages. 1982. (out of print)

Vol. 33: G.A. Martynov, R.R. Salem, Electrical Double Layer at a Metal-dilute Electrolyte Solution Interface. VI, 170 pages. 1983.

Vol. 34: N.D. Epiotis, Unified Valence Bond Theory of Electronic Structure ' Applications. VIII, 585 pages. 1983.

Vol. 35: Wavefunctions and Mechanisms from Electron Scattering Processes. Edited by F.A. Gianturco and G. Stefani. IX, 279 pages. 1984.

Vol. 36: J. Ugi, J. Dugundji, R. Kopp and D. Marquarding, Perspectives in Theoretical Stereochemistry. XVII, 247 pages. 1984.

Vol. 37: K. Rasmussen, Potential Energy Functions in Conformational Analysis. XIII. 231 pages. 1985.

Vol. 38: E. Lindholm, L. Åsbrink, Molecular Orbitals and their Energies, Studied by the Semiempirical HAM Method. X, 288 pages. 1985.

Vol. 39: P. Vany´sek, Electrochemistry on Liquid/Liquid Interfaces. 2, 3–108 pages. 1985.

Vol. 40: A. Plonka, Time-Dependent Reactivity of Species in Condensed Media. V, 151 pages. 1986.

Vol. 41: P. Pyykkö, Relativistic Theory of Atoms and Molecules. IX, 389 pages. 1986.

Vol. 42: W. Duch, GRMS or Graphical Representation of Model Spaces. V, 189 pages. 1986.

Vol. 43: F.M. Fernández, E.A. Castro, Hypervirial Theorems. VIII, 373 pages. 1987.

Vol. 44: Supercomputer Simulations in Chemistry. Edited by M. Dupuis. V, 312 pages. 1986.

Vol. 45: M.C. Böhm, One-Dimensional Organometallic Materials. V, 181 pages. 1987.

Vol. 46: S.J. Cyvin, I. Gutman, Kekulé Structures in Benzenoid Hydrocarbons. XV, 348 pages. 1988.

Vol. 47: C.A. Morrison, Angular Momentum Theory Applied to Interactions in Solids. 8,9–159 pages. 1988.

Vol. 48: C. Pisani, R. Dovesi, C. Roetti, Hartree-Fock Ab Initio Treatment of Crystalline Systems. V, 193 pages. 1988.

Vol. 49: E. Roduner, The Positive Muon as a Probe in Free Radical Chemistry. VII, 104 pages. 1988.

Vol. 50: D. Mukherjee (Ed.), Aspects of Many-Body Effects in Molecules and Extended Systems. VIII, 565 pages. 1989.

Vol. 51: J. Koca, M. Kratochvíl, V. Kvasnicka, L. Matyska, J. Pospíchal. Synthon Model of Organic Chemistry and Synthesis Design. VI, 207 pages. 1989.

Vol. 52: U. Kaldor (Ed.), Many-Body Methods in Quantum Chemistry. V, 349 pages. 1989.

Vol. 53: G.A. Arteca, F.M. Fernández, E.A. Castro, Large Order Perturbation Theory and Summation Methods in Quantum Mechanics. XI, 644 pages. 1990.

Vol. 54: S.J. Cyvin, J. Brunvoll, B.N. Cyvin, Theory of Coronoid Hydrocarbons. IX, 172 pages. 1991.

Vol. 55: L.T. Fan, D. Neogi, M. Yashima. Elementary Introduction to Spatial and Temporal Fractals. IX, 168 pages. 1991.

Vol. 56: D. Heidrich, W. Kliesch, W. Quapp, Properties of Chemically Interesting Potential Energy Surfaces. VIII, 183 pages. 1991.

Vol. 57: P. Turq, J. Barthel, M. Chemla, Transport, Relaxation, and Kinetic Processes in Electrolyte Solutions. XIV, 206 pages. 1992.

Vol. 58: B. O. Roos (Ed.), Lecture Notes in Quantum Chemistry. VII, 421 pages. 1992.

Vol. 59: S. Fraga, M. Klobukowski, J. Muszynska, E. San Fabian, K.M.S. Saxena, J.A. Sordo, T.L. Sordo, Research in Atomic Structure. XII, 143 pages. 1993.

Vol. 60: P. Pyykkö, Relativistic Theory of Atoms and Molecules II. A Bibliography 1986-1992. VIII, 479 pages. 1993.

Vol. 61: D. Searles, E. von Nagy-Felsobuki, Ab Initio Variational Calculations of Molecular Vibrational-Rotational Spectra. IX, 186 pages. 1993.

Vol. 62: S. J. Cyvin, J. Brunvoll, R. S. Chen, B. N. Cyvin F. J. Zhang, Theory of Coronoid Hydrocarbons II. XII, 310 pages. 1994.

Vol. 63: S. Fliszár, Atoms, Chemical Bonds and Bond Dissociation Energies. VIII, 173 pages. 1994.

Vol. 64: B. O. Roos (Ed.), Lecture Notes in Quantum Chemistry II. VII, 340 pages. 1994.

Vol. 65: R. O. Ponec, Overlap Determinant Method in the Theory of Pericyclic Reactions. VIII, 126 pages. 1995.

Vol. 66: S. Fraga, J. M. R. Parker, J. M. Pocock, Computer Simulations of Protein Structures and Interactions. XII, 282 pages. 1995.

Vol. 67: C. Pisani (Ed.), Quantum-Mechanical Ab-initio Calculation of the Properties of Crystalline Materials. VII, 328 pages. 1996.

Editorial Policy

This series aims to report new developments in chemical research and teaching - quickly, informally and at a high level. The type of material considered for publication includes:

1. Preliminary drafts of original papers and monographs
2. Lectures on a new field, or presenting a new angle on a classical field
3. Seminar work-outs
4. Reports of meetings, provided they are
   a) of exceptional interest and
   b) devoted to a single topic.

Texts which are out of print but still in demand may also be considered if they fall within these categories.

The timeliness of a manuscript is more important than its form, which may be unfinished or tentative. Thus, in some instances, proofs may be merely outlined and results presented which have been or will later be published elsewhere. If possible, a subject index should be included. Publication of Lecture Notes is intended as a service to the international chemical community, in that a commercial publisher, Springer-Verlag, can offer a wider distribution to documents which would otherwise have a restricted readership. Once published and copyrighted, they can be documented in the scientific literature.

Manuscripts

Manuscripts should comprise not less than 100 and preferably not more than 500 pages. They are reproduced by a photographic process and therefore must be typed with extreme care. Symbols not on the typewriter should be inserted by hand in indelible black ink. Corrections to the typescript should be made by pasting the amended text over the old one, or by obliterating errors with white correcting fluid. Authors receive 50 free copies and are free to use the material in other publications. The typescript is reduced slightly in size during reproduction; best results will not be obtained unless the text on any one page is kept within the overall limit of 18 x 26.5 cm (7 x $10^{1}/_{2}$ inches). The publishers will be pleased to supply on request special stationary with the typing area outlined.

Manuscripts should be sent to one of the editors or directly to Springer-Verlag, Heidelberg.