

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)

322APPENDIX A. SCHEDULE OF THE 1994 GICC SCHOOL OF COMPUTATIONAL CHEMISTRY

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

- acceleration techniques 68, 159
- acoustic mode 216
- adsorption, see chemisorption
- adjoined Gaussian 126
- alkali halides 184, 185, 192, 204
- aluminium 173
 - oxide 184, 186, 193
- angular integration 98
- anomalous dispersion (in diffraction) 260
- anti-ferromagnetic materials 109, 150, 197, 201, 292
- asymmetric unit 19
- atomic forces 148
- atomic orbital 126
- atomic partition method 92
- atomic units 48
- atomic weight function 93
- atomic sphere approximation 141
- Aufbau and anti-Aufbau 41, 141
- augmented plane wave 69
 - (full-potential) linearised 49, 139-153
- augmented spherical wave 141

- Bachelet, Hamann and Schlüter pseudopotentials 156
- band gap 39, 110, 157
- band structure 39, 170, 173, 176
 - projected 233, 241-243
 - two-dimensional 231
- Bardeen, Cooper and Schrieffer states 293
- basis lattice vectors 1
- basis set 61, 157, 181
 - criteria for selection 133
 - effects on results 181, 190, 195-199
 - incompleteness 64, 157
 - superposition error 64, 134
- Becke integration technique 92
- Berry phase 280-282
- beryllium 150
 - oxide 184
- bipolar expansion of two-electron integrals 130
- Bloch theorem 33
- Bloch function 35, 37, 126, 254
- Born effective charge tensor 274, 275
- Born-Haber cycle 203
- Born (or dynamical) matrix 216
- Born-Mayer (or Buckingham) potential 212
- Born-Oppenheimer approximation 47, 209, 276
- Born-Von Karman boundary conditions 36
- branches (of phonon dispersion relation) 216
- Bravais lattice 12
- Brillouin zone, first 18, 33, 215
 - sampling 157, 200
- bugs in programs 181
- bulk modulus 168, 191-195, 201

- calcium
 - carbonate 184, 186, 193, 223, 224
 - fluoride 218
 - oxide 184, 186, 193
- Car-Parrinello technique 69, 212
- cell
 - multiple or centred 3, 15
 - primitive 2
 - unit 2
 - Wigner-Seitz 17
- CETEP code 118
- Chadi-Cohen special point technique 81
- charge density, see position density
- chemisorption 234
 - energy 237
- Clausius-Mossotti 273
- cluster linearization scheme 292, 312
- cluster model of surfaces and defects 228
- cobalt oxide 149
- Compton profile 259, 261-263

- Compton scattering 256, 259
 computer performance 114
 copper oxide 150
 correlation of electronic motions 56, 58, 71,
 180, 249
 density functional expressions 58, 134,
 180-185, 193-195, 238
 in the electron gas 52
 interionic 194
 intra-atomic 194
 Coulomb hole 254
 Coulomb series 128
 counterpoise technique 64
 coupled-cluster techniques 58
 coupled Hartree-Fock methods 285
 CRYSTAL code 91, 125-137, 179-207, 236,
 238, 245, 253
 parallelization 115
 crystalline orbital 32, 65, 126, 144
 system 11
 crystallographic
 axes 2
 directions 4
 planes 4
 current density 274, 279
 cutoff (in PW expansion) 61, 160, 168-175

 Debye temperature 203
 defect 227-244
 charged 236
 formation energy 183, 238
 state 237
 density functional theory 53, 91, 140, 158,
 180, 212, 220, 254
 density matrix 49, 245-272
 eigenvalues and eigenfunctions 248
 reconstruction 256, 268
 density of states 44, 52, 66
 Fourier-Legendre expansion 67, 132
 integrated 66
 projected 44, 66, 69, 132
 density of vibrational states 222
 density operator 252
 dielectric polarization 273-288
 dielectric tensor 274, 286
 dipole moment derivatives 275
 disordered systems 211
 dispersion forces 183, 185, 194, 213
 dispersion relation (phonon) 216
 displacement polar tensor 275
 distributed data approach 118
 distributed memory 115

 dynamical matrix 216

 elastic constants 191-193, 214
 electric field gradient 146, 150
 electron diffraction 256, 258
 electron gas 51
 electron-phonon coupling 293
 electrostatic effects 184, 186
 embedding techniques 230
 enantiomorphic objects 7, 10
 energy
 binding 193-195
 derivatives 148, 180, 193-195
 electronic, per unit cell 127, 179-207
 minimization 149, 210
 vibrational 221
 ensemble
 canonical (NpT) 211,
 constant pressure (NpH) 211,
 constant pressure canonical (NpT) 211,
 microcanonical (NVE) 211, 247
 enthalpy 188
 of formation 203
 entropy 222
 equation of state 169, 187, 210
 equilibrium geometry, see lattice parameter
 exchange-correlation functional 53, 140
 exchange hole 254
 exchange series 129
 extinction (in diffraction experiments) 257
 extracule coordinates 250

 fast Fourier transform 120, 161
 Fermi energy 45, 66, 87, 158
 Fermi surface 45, 87, 157
 fermionic linearization 312
 ferro-antiferromagnetic transition 197, 201
 ferroelectric crystal 274
 force constants 212
 form factor 256-258, 260
 Fourier transform 79, 161
 Fourier-Dirac transformation 251
 fractional coordinates 3
 free energy (Gibbs) 188
 frozen core approximation 156
 frozen nuclear motion, see static lattice energy
 fullerene 301
 full-potential, see augmented plane wave

 Gaussian type orbital 61, 122
 Gauss-Laguerre quadrature 97
 Gauss-Legendre quadrature 97

- generalised gradient approximation, see
 gradient-corrected functional
 geometric (quantum) phase, see Berry phase
 geophysics 187
 Gilat net 132
 global summation 116
 gradient-corrected functional 56, 58, 141
 Green-function techniques 58, 68–71, 229,
 239–241
 Grueneisen parameter 223

 halides 184–192
 harmonic approximation 214–216
 harmonic potential, see model potential
 Hartree-Fock 51, 56–59, 125–137, 179–207,
 219, 276–278
 in dielectric polarization theory 273–288
 eigenvalues 58
 energy 193–195
 orbitals and density matrix 249
 heat capacity 222
 Hellmann-Feynmann
 force 148
 theorem 279
 Helmholtz free energy 222
 hopping
 amplitude 290
 exchange process 291
 pair process 291
 Hubbard models 289–319
 hybrid HF/DFT method, 91

 ideal surface, see surface
 idempotency of one-matrices 249
 ilmenite 189, 198
 indices
 of plane (Miller indices) 5
 of row 4
 indium 150
 inelastic scattering 256, 259–260
 infrared charges 275
 infrared vibrational spectra 217
 integrals (two-electron) 127
 interstitial region 142
 intracule coordinates 250
 ionic conductors 211
 iron 149, 13
 oxide 186
 fluoride 149
 irreducible representation 32
 itinerant interacting electrons 290, 292, 299

 Jastrow factor 71

 Korringa-Kohn-Rostoker technique 68
 Kohn-Sham
 equations, see density functional theory
 orbitals 254
 Kubo formula 279

 lattice
 constant 2, 168
 direct 6
 dynamics 209–225, 274
 nodes 2
 parameter (calculated) 184–186
 reciprocal 6, 32
 sums 106, 128, 129
 Laue classes 11
 Lebedev grid 98
 linear dependence catastrophe 63, 133, 199
 linear response methods 274, 285
 lithium
 halides 184, 185, 192, 204
 nitride 150
 oxide 193
 load balancing 115
 local approach 59
 local defect, see defect
 local density approximation 54, 140, 156
 local orbital 144
 local spin density approximation 101, 140
 localised orbitals, see Wannier functions

 macroscopic bulk observable 276
 magnesium
 carbonate 184, 186, 193
 oxides 184, 186, 189, 193, 198
 silicate 186–191, 198
 magnetic properties 109, 148, 149, 197
 manganese
 fluoride (KMnF_3) 150, 195–197, 201
 oxide 186
 mercury halides 150
 metal-insulator transition 292
 metastable configurations 210
 metric tensor or matrix 5, 6
 model potential 212–216
 Moeller-Plesset method 58
 molecular crystals 151
 molecular dynamics 211
 momentum density 256, 266
 Monkhorst net 132
 Monkhorst-Pack special points 81

- Montecarlo techniques 70
 Morse potential, see model potential
 Mott-Hubbard transition 292, 312
 Mott insulator 149
 Moyal density function 251
 muffin-tin approximation 68, 142
 multiple diffraction 260
 multi-slab model 230
 Murnaghan equation 169
- natural spin geminals 248
 natural spin orbitals 248
 Neumann principle 11
 neutron diffraction 256, 261
 neutron scattering vibrational spectra 217
 nickel
 halides 149, 150
 oxide 186
 non-Euclidean lattices 299
 tesselation 302
 normal modes (of vibration) 211, 215
 norm-conserving pseudopotentials 156
 N-scaling techniques 71
 nuclear quadrupole interaction
 constant 150
 numerical approximations 181, 199-202
 numerical integration 91-100
- observable (ground-state
 expectation value) 71, 134
 phase-dependent 278
 off-diagonal long-range order eigenstate 293
 one-matrix, see density matrix
 open-shell systems 102
 optic mode 216
 origin (choice of) 26
 oxides 183-195
- parallel processor 115
 PARAPOCS code 224
 periodic boundary conditions 36, 216
 perovskites 149, 187, 198
 phase space density 250
 phase transition 149, 189
 phonon 218, 220
 field 293
 transverse optic 275
 piezoelectric tensor 274
 plane wave 61, 142, 156
 point group 9, 79
 Poisson equation 62, 276
 polarizability 186
- polarization 185
 derivative or difference 274
 linear response approach 274, 287
 theory 273-288
 zero-field 274-276
 polarization functions 197
 Pople-Nesbet equations 103
 position density 256
 potassium
 fluoride (KMnF_3) 195-197, 201
 halides 184, 185, 192, 204
 oxide 198
 potential energy surface (or function) 210
 pressure (vibrational) 223
 pseudo-potentials 59, 156, 181, 196
 PWSCF code 78, 155-178
- quartz (α) 186, 214
 quasi-harmonic model 223
- radial integration 97
 Raman vibrational spectra 217
 reciprocal form factor 256, 263-266
 reciprocal space integration 66, 77-89, 132
 recursion technique 69
 reduced density matrices 248
 relativistic effects 48, 62, 141, 146
 repeat(ing) unit 1
 (in crystalline slabs) 231
 replicated data approach 115
 residual instrumental function 263
 restricted open-shell Hartree-Fock 102
 rigid ion model 224
 rubidium halides 184, 185, 192
- scalar-relativistic approximation 141
 scattering experiments 256, 258-263
 screened macroscopic field 287
 self-consistent-field procedure 54, 67, 135,
 147, 159
 self-interaction correction 56
 semiconductors (IV-IV, III-V) 183, 185, 192,
 220
 setting (in space groups) 17, 19
 shared memory 114
 shell model 213, 224
 silicon 86, 167, 183, 185, 220
 oxide 186, 214
 (111) surface 234
 slab model 230
 Slater type orbital 62
 sodium

- chloride 171, 182, 203
- halides 184, 185, 192, 204
- oxide 198
- space group 18, 78
 - symmorphic, non-symmorphic 21
- special point techniques 66, 77-89, 161, 176
- spin density 104, 256
 - in momentum space 263
- spin eigenfunction 102
- spin-free density matrices 252
- static lattice energy 188, 203
- statistical mechanics 212
- stishovite 189, 198
- structure factor, see form factor
- supercell 183, 219, 231, 236-239
- superconductivity (high T_c) 289-319
- superconductor (high T_c) 149, 150
- surface (crystalline) 227-244
 - formation energy 229, 237
 - of ionic crystals 231
 - relaxation 229, 237
 - reconstruction 229, 237
 - stability 231
 - state 231
- symmetry
 - axis (rotation, rotoinversion, screw) 8, 9
 - class 9
 - element 7
 - exploitation 131, 156
 - inversion 9
 - operation (proper, improper) 9, 10
 - plane (reflection and glide) 8
 - translational 1
- synchronous global index 115
- Tasker type (of ionic surface) 231
- temperature effects 203, 209-225
- tetrahedron method 67, 87
- thermodynamic functions 221
- thermodynamic properties 209-225
- three-body potential, see model potential
- tight-binding scheme 289
- titanium oxide 150
- transition metal compounds 109, 150, 186
- travelling wave 215
- triangular groups (elliptic, hyperbolic) 302
- two-body potential, see model potential
- unrestricted Hartree-Fock 103
- urea 199
- vector processor 115
- velocity operator 277
- vibration modes, see normal modes
- vibrational spectroscopy 217
- virial theorem 266
- visualization 121
- Voronoi polyhedron (cell) 17, 93
- Wannier functions 254
- Wigner density function 251
- Wigner-Seitz cell 17
- WIEN code 139-153
- X-ray diffraction 256, 258-259
- zero-point energy 203
- zinc 150

Appendix C

List of Acronyms

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

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