A

Matrices of the Symmetrical Supercell Transformations of 14 Three-dimensional Bravais Lattices

A.1. The triclinic crystal system
(i) l(P,P) is an arbitrary integer matrix.

A.2. The monoclinic crystal system

(i) $l(\mathrm{P,P}) = \begin{pmatrix} n_1 & n_5 & 0 \\ n_4 & n_2 & 0 \\ 0 & 0 & n_3 \end{pmatrix}, \qquad L = (n_1 n_2 - n_4 n_5) n_3;$ (A.1)

(ii) $l(\mathrm{A,P}) = \begin{pmatrix} n_1 & n_5 & 0 \\ n_4 & n_2 & -n_3 \\ n_4 & n_2 & n_3 \end{pmatrix}, \qquad L = 2(n_1 n_2 - n_4 n_5) n_3;$

(iii) $l(\mathrm{P,A}) = \begin{pmatrix} n_1 & n_4 & n_4 \\ n_5 & n_2 & n_2 \\ 0 & -n_3 & n_3 \end{pmatrix}, \qquad L = 2(n_1 n_2 - n_4 n_5) n_3;$

(iv) $l(\mathrm{A,A}) = \begin{pmatrix} n_1 & n_5 & n_5 \\ n_4 & n_2 + n_3 & n_2 - n_3 \\ n_4 & n_2 - n_3 & n_2 + n_3 \end{pmatrix}, \qquad L = 4(n_1 n_2 - n_4 n_5) n_3;$

A.3. The hexagonal crystal system

(i) $l^{(1)}(\mathrm{P,P}) = \begin{pmatrix} n_1 & 0 & 0 \\ 0 & n_1 & 0 \\ 0 & 0 & n_2 \end{pmatrix}, \qquad L = n_1^2 n_2;$ (A.2)

(ii) $l^{(2)}(\mathrm{P,P}) = \begin{pmatrix} n_1 & -n_1 & 0 \\ n_1 & 2n_1 & 0 \\ 0 & 0 & n_2 \end{pmatrix}, \qquad L = 3n_1^2 n_2;$

A.4. The rhombohedral crystal system

(i) $l(\mathrm{R,R}) = \begin{pmatrix} n_1 + n_2 & n_2 & n_2 \\ n_2 & n_1 + n_2 & n_2 \\ n_2 & n_2 & n_1 + n_2 \end{pmatrix}, \qquad L = n_1^2 (n_1 + 3n_2);$

A.5. The orthorhombic crystal system

(i) l(P,P) coincides with (A.1);

(ii) $l(\mathrm{C,P}) = \begin{pmatrix} n_1 & -n_2 & 0 \\ n_1 & n_2 & 0 \\ 0 & 0 & n_3 \end{pmatrix}$, $L = 2n_1n_2n_3$;

(iii) $l(\mathrm{F,P}) = \begin{pmatrix} 0 & n_2 & n_3 \\ n_1 & 0 & n_3 \\ n_1 & n_2 & 0 \end{pmatrix}$, $L = 2n_1n_2n_3$;

(iv) $l(\mathrm{I,P}) = \begin{pmatrix} -n_1 & n_2 & n_3 \\ n_1 & -n_2 & n_3 \\ n_1 & n_2 & -n_3 \end{pmatrix}$, $L = 4n_1n_2n_3$;

(v) $l(\mathrm{P,C}) = \begin{pmatrix} n_1 & n_1 & 0 \\ -n_2 & n_2 & 0 \\ 0 & 0 & n_3 \end{pmatrix}$, $L = 2n_1n_2n_3$;

(vi) $l(\mathrm{C,C}) = \begin{pmatrix} n_1 & n_2 & 0 \\ n_2 & n_1 & 0 \\ 0 & 0 & n_3 \end{pmatrix}$, $L = (n_1^2 - n_2^2)n_3$;

(vii) $l(\mathrm{A,C}) = \begin{pmatrix} n_1 & n_1 & 0 \\ -n_2 & n_2 & -n_3 \\ -n_2 & n_2 & n_3 \end{pmatrix}$, $L = 4n_1n_2n_3$;

(viii) $l(\mathrm{F,C}) = \begin{pmatrix} -n_2 & n_2 & n_3 \\ n_1 & n_1 & n_3 \\ n_1 - n_2 & n_1 + n_2 & 0 \end{pmatrix}$, $L = 4n_1n_2n_3$;

(ix) $l(\mathrm{I,C}) = \begin{pmatrix} -n_1 & -n_2 & n_3 \\ n_1 & n_2 & n_3 \\ n_2 & n_1 & -n_3 \end{pmatrix}$, $L = 2(n_1^2 - n_2^2)n_3$;

(x) $l(\mathrm{P,F}) = \begin{pmatrix} -n_1 & n_1 & n_1 \\ n_2 & -n_2 & n_2 \\ n_3 & n_3 & -n_3 \end{pmatrix}$, $L = 4n_1n_2n_3$;

(xi) $l(\mathrm{C,F}) = \begin{pmatrix} -n_1 & n_1 & n_2 \\ -n_2 & n_2 & n_1 \\ n_3 & n_3 & -n_3 \end{pmatrix}$, $L = 2(n_1^2 - n_2^2)n_3$;

(xii) $l(\mathrm{F,F}) = \frac{1}{2}\begin{pmatrix} n_2 + n_3 & -n_2 + n_3 & n_2 - n_3 \\ -n_1 + n_3 & n_1 + n_3 & n_1 - n_3 \\ -n_1 + n_2 & n_1 - n_2 & n_1 + n_2 \end{pmatrix}$, $L = n_1n_2n_3$; n_1, n_2, n_3 are of the same parity;

(xiii) $l(\mathrm{I,F}) = \begin{pmatrix} n_1 + n_2 + n_3 & -n_3 & -n_2 \\ -n_3 & n_1 + n_2 + n_3 & -n_1 \\ -n_2 & -n_1 & n_1 + n_2 + n_3 \end{pmatrix}$,

$L = 2[(n_1 + n_2 + n_3)(n_1n_2 + n_2n_3 + n_3n_1) - n_1n_2n_3]$;

(xiv) $l(\mathrm{P,I}) = \begin{pmatrix} 0 & n_1 & n_1 \\ n_2 & 0 & n_2 \\ n_3 & n_3 & 0 \end{pmatrix}$, $L = 2n_1n_2n_3$;

(xv) $l(\mathrm{C,I}) = \begin{pmatrix} -n_2 & n_1 & n_1 - n_2 \\ n_2 & n_1 & n_1 + n_2 \\ n_3 & n_3 & 0 \end{pmatrix}$, $L = 4n_1n_2n_3$;

(xvi) l(F,I)= $\begin{pmatrix} n_2+n_3 & n_3 & n_2 \\ n_3 & n_1+n_3 & n_1 \\ n_2 & n_1 & n_1+n_2 \end{pmatrix}$, $L = 4n_1n_2n_3$;

(xvii) l(I,I)= $\frac{1}{2}\begin{pmatrix} n_2+n_3 & -n_1+n_3 & -n_1+n_2 \\ -n_2+n_3 & n_1+n_3 & n_1-n_2 \\ n_2-n_3 & n_1-n_3 & n_1+n_2 \end{pmatrix}$, $L = n_1n_2n_3$; n_1, n_2, n_3 are of the same parity;

A.6. The tetragonal crystal system

(i) $l^{(1)}$(P,P) coincides with (A.2);

(ii) $l^{(2)}$(P,P)= $\begin{pmatrix} n_1 & -n_1 & 0 \\ n_1 & n_1 & 0 \\ 0 & 0 & n_2 \end{pmatrix}$, $L = 2n_1^2n_2$;

(iii) $l^{(1)}$(I,P)= $\begin{pmatrix} 0 & n_1 & n_2 \\ n_1 & & n_2 \\ n_1 & n_1 & 0 \end{pmatrix}$, $L = 2n_1^2n_2$;

(iv) $l^{(2)}$(I,P)= $\begin{pmatrix} -n_1 & n_1 & n_2 \\ n_1 & -n_1 & n_2 \\ n_1 & n-1 & -n_2 \end{pmatrix}$, $L = 4n_1^2n_2$;

(v) $l^{(1)}$(P,I)= $\begin{pmatrix} 0 & n_1 & n_1 \\ n_1 & 0 & n_1 \\ n_2 & n_2 & 0 \end{pmatrix}$, $L = 2n_1^2n_2$;

(vi) $l^{(2)}$(P,I)= $\begin{pmatrix} -n_1 & n_1 & 0 \\ n_1 & n_1 & 2n_1 \\ n_2 & n_2 & 0 \end{pmatrix}$, $L = 4n_1^2n_2$;

(vii) $l^{(1)}$(I,I)= $\begin{pmatrix} n_1+n_2 & n_2 & n_1 \\ n_2 & n_1+n_2 & n_1 \\ n_1 & n_1 & 2n_1 \end{pmatrix}$ $L = 4n_1^2n_2$;

(viii) $l^{(2)}$(I,I)= $\frac{1}{2}\begin{pmatrix} n_1+n_2 & -n_1+n_2 & 0 \\ -n_1+n_2 & n_1+n_2 & 0 \\ n_1-n_2 & n_1-n_2 & 2n_1 \end{pmatrix}$ $L = n_1^2n_2$; n_1, n_2 are of the same parity;

A.7. The cubic crystal system

(i) l(P,P)=l(F,F)=l(I,I)= $\begin{pmatrix} n & 0 & 0 \\ 0 & n & 0 \\ 0 & 0 & n \end{pmatrix}$, $L = n^3$;

(ii) l(F,P)=l(P,I)= $\begin{pmatrix} 0 & n & n \\ n & 0 & n \\ n & n & 0 \end{pmatrix}$, $L = 2n^3$;

(iii) l(I,P)=l(P,F)= $\begin{pmatrix} -n & n & n \\ n & -n & n \\ n & n & -n \end{pmatrix}$, $L = 4n^3$;

(iv) l(I,F)= $\begin{pmatrix} 3n & -n & -n \\ -n & 3n & -n \\ -n & -n & 3n \end{pmatrix}$, $L = 16n^3$;

(v) l(F,I)= $\begin{pmatrix} 2n & n & n \\ n & 2n & n \\ n & n & 2n \end{pmatrix}$, $L = 4n^3$.

B

Reciprocal Matrices of the Symmetric Supercell Transformations of the Three Cubic Bravais Lattices

$$Q_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad Q_2 = \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix} \quad Q_3 = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

$$Q_4 = \begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix} \quad Q_5 = \begin{pmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{pmatrix}$$

C

Computer Programs for Periodic Calculations in Basis of Localized Orbitals

The information about computer programs applied in molecular quantum chemistry and materials science can be found on different Internet sites [856–858]. In particular, on site [856] on-line links are given to the appropriate information. The majority of the existing computer codes for calculations of periodic systems can be divided into two main groups: LO codes using a basis set of localized orbitals (LO) and PW(APW) codes using plane waves (PW) or augmented plane waves (APW) as a basis set. The only exclusion is the hybrid Gaussian LO and PW (GPW) DFT code QUICKSTEP/CP2K [859]. The sites mentioned include references to both LO and PW codes. The information about periodic codes using LO or PW bases can also be found in [568, 860]. Here, we restrict ourselves only to brief information about computer codes for periodic LO calculations (see Table C.1). The indication of the corresponding homepage and references on the publications are given in the last two columns of Table C.1. Both ab-initio (HF,DFT (LDA,GGA), hybrid HF-DFT, time-dependent DFT (TDFT)) and semi-empirical (SE) codes are included in the list. The codes listed allow all-electron (AE) calculations (also termed full potential-FP) or valence-only ones with the use of pseudopotential (PP) for core electrons or both. For the localized basis we use the acronyms GTO (Gaussian-type orbitals), STO (Slater-type orbitals) and NTO (numerical type orbitals). In particular, f-GTO and f-polarization-GTO mean the possibility to make full GTO calculations for f-elements or the simple extension of Gaussian basis-sets to include f-polarization basis-functions, respectively. In the remaining cases only s, p and d orbitals can be used in the basis set. The geometry optimization can be made over the atomic coordinates only (GO) or including both the lattice parameters optimization (full GO). Some codes allow linear scaling ($O(N)$) with the basis-set size and molecular-dynamics (MD) calculations. The semiempirical codes can allow the band structure calculations for nonzero wave vectors (BAND) or the cyclic-cluster model (CCM) without the BZ summation can be used. The CRYSTAL suite remains the mostly advanced and developing LCAO periodic program, compared to other codes listed in Table C.1. We refer the reader to the calculations of metal-organic frameworks (MOF), [872] as a case study showing that the CRYSTAL program allows reliable *ab-initio* prediction of materials properties of complex systems to be made. Note that from January 1st, 2007, CRYSTAL03 will not be supported any more.

Table C.1. List of periodic computer programs using localized orbitals basis

No	Program	Description	Web site	Refs
1	CRYSTAL03	HF;DFT (LDA,GGA); Hybrid HF-DFT; AE; PP; GTO; GO	www.crystal.unito.it www.cse.clrc.ac.uk/cmg	[568, 860–863]
2	CRYSTAL06	+ f-polarization-GTO, full GO, vibrational frequences	www.crystal.unito.it/ home.html	
3	CRYSCOR	+ MP2 correlation	www.crystal.unito.it	[201]
4	GAUSSIAN03	HF;DFT (LDA,GGA); PHF; Hybrid HF-DFT; AE; PP;f-GTO; GO;O(N)	www.gaussian.com	[379]
5	ADF2006 (BAND)	DFT (LDA,GGA); Hybrid HF-DFT; TD-DFT; AE; STO;	/www.scm.com/Doc/ Doc2006.01	[864]
6	SIESTA	DFT (LDA,GGA);PP; NTO; GO; MD ;O(N)	www.uam.es/ departamentos/ ciencias/ fismateriac/siesta	[400]
7	AIMPRO	DFT(LDA,GGA); PP; LGTO	http://newton/ex/ ac.uk/research	[555]
8	SEQUEST	DFT (LDA, GGA);PP; GTO;O(N);GO	http://dft.sandia. gov/Quest	[865]
9	DMOL3	DFT (LDA, GGA);AE; NTO; GO	http://people.web.psi.ch/ delley/dmol3.html	[866]
10	FPLO	DFT (LSDA,LSDA+U); AE; LO;	www.fplo.de	[867]
11	PLATO	DFT (LDA); NTO;GO	www-staff.lboro.ac.uk / masdk/plato.html	[868]
12	QUICKSTEP/ CP2K	DFT(LDA,GGA); PP;GTO/PW	http://cp2k.berlios.de	[859]
13	CNDO 4.0	SE,BAND,GE	www.wgc.chem.pu.ru / valera/cndo/manual.html	[869]
14	MOPAC2002	SE,BAND,GE	www.cachesoftware. com/mopac	[312, 870]
15	MSINDO	SE,CCM,STO,GO,MD	www.theochem. uni-hannover.de/ Bredow/MSINDO	[256]
16	SOLID2000	SE,CCM,QR-INDO, STO,GO	www.stech.sk/stech soft/htm	[307]
17	SYM-SYM	SE,CCM,INDO,GO	www.cmmp.ucl.ac.uk / lev/recearc4/node8.html	[871]

The reader can also find useful such codes as XCrysDen([873], GULP([875] and BAND-GUI([345].

XCrysDen program can be used as a graphical user interface (GUI) for the CRYSTAL95/98/03/06 programs. The advantage of the GUI is its rendering possibility, which yields graphical feedback to the user. Every manipulation of the structure is visualized immediately and to enhance the usefulness of XCrySDen even further, an UNDO/REDO option is available, which makes every false move recoverable. Several graphical procedures make the manipulation of the atomic structures easier, while other graphical functions are suitable for checking the geometry of the structure. This program uses the ease of a GUI and the flexibility of manual editing and allows the user to view and edit the input scripts for the CRYSTAL programs on request. Immediately after the manual editing is completed the program visualizes the result. We refer the reader for details to the program description [874].

GULP is a program for performing a variety of types of simulation on materials using boundary conditions of 0D (molecules and clusters), 1D (polymers), 2D (surfaces, slabs and grain boundaries), or 3D (periodic solids). The focus of the code is on analytical solutions, through the use of lattice dynamics, where possible, rather than on molecular dynamics. A variety of force fields can be used within GULP spanning the shell model for ionic materials, molecular mechanics for organic systems, and the embedded-atom model for metals. Analytic derivatives are included up to at least second order for most force fields, and to third order for many.

ADF2006.01 is the first ADF release containing a graphical user interface for the BAND program. BAND input also enables inexperienced ADF-BAND users to easily create BAND jobs. You can use BAND input to define your periodic structure (geometry), and to set details of your BAND job using an easy-to-use graphical user interface. BAND input will generate the complete job script for you. This script takes care of running BAND. You can also use BAND input to run these script files on your local machine in the background.

References

1. R. Dronskowski, *Computational Chemistry of Solid State Materials. A Guide for Materials Scientists, Chemists, Physicists and Others* (Wiley-VCH, Weinheim, 2005)
2. C.M. Quinn, *An Introduction to Quantum Chemistry of Solids* (Clarendon Press, Oxford, 1973)
3. A.A. Levin, *Solid State Quantum Chemistry* (McGraw-Hill, New York, 1977)
4. *Ab-initio Calculations of the Properties of Crystalline Materials*, ed. C. Pisani, Lecture Notes in Chemistry **67** (Springer Verlag, Berlin, 1996)
5. P. Fulde, *Electron Correlations in Molecules and Solids*, 3rd edn. Springer Series in Solid State Sciences 100 (Springer, Berlin Heidelberg New York, 1995)
6. W. Harrison, *Electronic Structure and Properties of Solids: Physics of the Chemical Bond*, 2nd edn. (Dover, New York, 1989)
7. R. Hoffmann, *Solids and Surfaces: A Chemist View on Bonding in Extended Structures* (Weinheim VCH, 1988)
8. M. Springborg, *Methods of Electronic Structure Calculations* (Wiley, 2000)
9. E. Kahiras, *Atomic and Electronic Structure of Solids* (Cambridge University Press, Cambridge, 2003)
10. R. Martin, *Electronic Structure. Basic Theory and Practical Methods* (Cambridge University Press, Cambridge, 2004)
11. L. Kantorovich, *Quantum Theory of the Solid State* (Kluwer Academic Publishers, Dordrecht, 2004)
12. K. Ohno, R. Esfarjani, Y. Kawazoe, *Computational Materials Science*, Springer Series in Solid State Sciences, **129** (Springer, Berlin Heidelberg New York, 1999)
13. R.A. Evarestov, V.P. Smirnov, *Site Symmetry in Crystals: Theory and Applications*, 2nd edn. Springer Series in Solid State Sciences, **108** (Springer, Berlin Heidelberg New York, 1997)
14. R.L. Flurry, *Symmetry Groups. Theory and Chemical Applications* (Prentice-Hall, Englewood Cliffs, NJ, 1980)
15. P.W.M. Jacobs, *Group Theory with Applications in Chemical Physics* (Cambridge University Press, New York, 2005)
16. *Bilbao Crystallographic Server*, http://www.cryst.ehu.es/
17. A.P. Cracknell, B.L. Davies, S.C. Miller, W.F. Love, *Kronecker Product Tables*, **1** *General Introduction and Tables of Irreducible Representations of Space Groups* (IFI/Plenum, New York-Washington-London, 1979)
18. M.I. Petrashen, E.D. Trifonov, *Applications of Group Theory in Quantum Mechanics* (M.I.T. Press, Massachusetts, 1969)

19. *International Tables for Crystallography*, ed. T.Hahn, **A** Space-group symmetry (Reidel, Dordrecht, 1983)
20. http://cst-www.nrl.navy.mil/lattice/
21. http://cst-www.nrl.navy.mil/lattice/others.html
22. Inorganic Crystal Structure Database (ICSD), http://www.fiz-informationsdienste.de/en/DB/icsd/
23. V.R. Saunders, R. Dovesi, C. Roetti, R. Orlando, C.M.Zicovich-Wilson, N.M.Harrison, CRYSTAL-2003 Users Manual, University of Torino, Torino, 2003; http://www.crystal.unito.it
24. Richard J.D. Tilley, *Crystals and Crystal Structures* (Wiley, 2006)
25. A. Munoz, J.A. Alonso, M.J. Martinez-Lope, M.T. Casais, J.L. Martinez, M.T. Fernandez-Diaz, Phys. Rev. B **62**, 6498 (2000)
26. John Z.H. Zhang, *Theory and Application of Quantum Molecular Dynamics* (World Scientific Publishing Co., Singapore, 1999)
27. G.L. Bir, G.E. Pikus, *Symmetry and Strain-induced Effects in Semiconductors* (Wiley, New York, 1972)
28. C. Zicovich-Wilson, R. Dovesi, Int. J. Quantum Chem. **67**, 299 (1998)
29. C. Zicovich-Wilson, R. Dovesi, Int. J. Quantum Chem. **67**, 311 (1998)
30. C.J. Bradley, A.P. Cracknell, *The Mathematical Theory of Symmetry in Solids* (Clarendon, Oxford, 1972)
31. O.V. Kovalev, *Representations of the Crystallographic Space Groups: Irreducible Representations, Induced Representations and Corepresentations*, 2nd edn. ed. by H.T. Stokes, D.M. Hatch (Gordon and Breach, Philadelphia, PA 1993)
32. I. Shur, J.F.Math. **139**, 155 (1911)
33. G.Ya. Lyubarskii, *The Application of Group Theory in Physics* (Pergamon, Oxford, 1960)
34. C.Herring, J. Franklin Inst. **233**, 525 (1942)
35. M.W. Schmidt, K.K. Baldridge, J.A. Boatz, S.T. Elbert, M.S. Gordon, J.H. Jensen, S. Koseki, N. Matsunaga, K.A. Nguyen, S. Su, T.L. Windus, M. Dupuis, J.A.J.Jr. Montgomery, J. Comput. Chem. **14**, 1347 (1993)
36. C. Edmiston, K. Ruedenberg, Rev. Mod. Phys. **35**, 457 (1963)
37. J. Pipek, P.G. Mezey, J. Chem. Phys. **90**, 4916 (1989)
38. S.F. Boys, Rev. Mod. Phys. **32**, 296 (1960)
39. J. Zak, Phys. Rev. B **23**, 2824 (1981)
40. H. Bacry, L. Michel, J. Zak, Lect. Notes Phys. **313**, 291 (Springer, Berlin, Heidelberg, 1988)
41. M. Schütz, G. Hetzer, H.-J. Werner, J. Chem. Phys. **111**, 5691 (1999)
42. V.P. Smirnov, D.E. Usvyat, Phys. Rev. B. **64**, 245108 (2001)
43. G. Wannier, Phys. Rev. **52**, 191 (1937)
44. W. Kohn, Phys. Rev. **115**, 809 (1959)
45. J. Des Cloizeaux, Phys. Rev. **135**, A698 (1964)
46. N. Marzari, D. Vanderbilt, Phys. Rev. B, **56**, 12847 (1997)
47. V.P. Smirnov, R.A. Evarestov, D.E. Usvyat, Int. J. Quantum. Chem. **88**, 642 (2002)
48. B. Sporkmann, H. Bross, Phys. Rev. B. **49**, 10869 (1994)
49. A. Shukla, M. Dolg, P. Fulde, H. Stoll, Phys. Rev. B. **60**, 5211 (1999)
50. S. Goedecker, Rev. Mod. Phys. **71** , 1085 (1999)
51. I. Souza, R.M. Martin, N. Marzari, X. Zhao, D. Vanderbilt, Phys. Rev. B. **62** , 15505 (2000)
52. P.Y. Yu, M. Cardona, *Fundamentals of Semiconductors. Physics and Materials Properties*, 3rd rev. and enlarged edn. (Springer, Berlin, Heidelberg, 2005)
53. C.M. Zicovich-Wilson, R. Dovesi, V.R. Saunders, J. Chem. Phys. **115**, 9708 (2001)
54. I. Mayer, G. Rather, S. Suhai, Chem. Phys. Lett. **293**, 81 (1998)

55. R.A. Evarestov, V.P. Smirnov, phys. stat. sol. (b) **180**, 411 (1993)
56. J. Des Cloizeaux, Phys. Rev. **129**, 554 (1963)
57. W. Kohn, Phys. Rev. B, **7**, 4388 (1973)
58. J.C. Slater, G.F. Koster, Phys.Rev. **94**, 1498 (1954)
59. V.P. Smirnov, D.E. Usvyat, Phys. Rev. B **59**, 9695 (1999)
60. N. Marzari, D. Vanderbilt, in *First-Principles Calculations for Ferroelectrics*, ed. R.E. Cohen, AIP Conf. Proc. No 436 (AIP, Woodbury, 1998), p.146
61. I. Souza, N. Marzari, D. Vanderbilt, Phys. Rev. B **65**, 035109 (2001)
62. http://www.wannier-transport.org
63. C.M. Zicovich-Wilson, A. Bert, C. Roetti, R. Dovesi, V.R. Saunders J. Chem. Phys. **116**, 1120 (2002)
64. A. Bert, M. Llunell, R. Dovesi, C.M. Zicovich-Wilson, Phys. Chem. Chem. Phys. **5**, 5319 (2003)
65. E. Clementi, C. Roetti, *Roothaan–Hartree–Fock Atomic Functions*, in Atomic Data and Nuclear Data Tables, **14**, 177 (1974)
66. C.C.J. Roothaan, Rev. Mod. Phys. **23**, 69 (1951)
67. C.C.J. Roothaan, Rev. Mod. Phys. **32**, 179 (1960)
68. J.A. Pople, R.K. Nesbet, J. Chem. Phys. **22**, 571 (1954)
69. E. Apra, Lecture Notes in Chem. **67**, 101 (1996)
70. R.A. Evarestov, I.I. Tupitsyn, Phys. Solid State **44**, 1656 (2002)
71. P.P. Ewald, Ann. Phys. **64**, 253 (1921)
72. A.B. Kunz, Phys. Rev. B **6**, 606 (1972)
73. J.J. Ladik, Phys. Rep. **313**, 171 (1999)
74. J.-M. Andre, L. Gouverneur, G. Leroy, Int. J. Quantum Chem. **1**, 427, 451 (1967)
75. C. Pisani, R. Dovesi, Int. J. Quantum Chem. **17**, 501, 517 (1980)
76. R. Dovesi, C. Pisani, C. Roetti, P.Dellarole, Phys. Rev. B **24**, 4170 (1981)
77. R. Dovesi, M. Causa, G. Angonoa, Phys. Rev. B **24**, 4177 (1981)
78. M. Causa, Lecture Notes in Chem. **67**, 91 (1996)
79. C. Pisani, U.Birkenheuer, Comp. Phys. Commun. **96**, 221 (1996)
80. http://www.crystal.unito.it
81. http://www.cse.clrc.ac.uk
82. K.N. Kudin, G.E. Scuseria, Phys. Rev. B **61**, 16440 (2000)
83. R. Improta, K.N. Kudin, G.E. Scuseria, V. Barone, J. Am. Chem. Soc **124**, 113 (2002)
84. N.W. Ashcroft, N.D. Mermin, *Solid State Physics* (Cole, London, 1976)
85. M.F. Guest, V.R. Saunders, Mol. Phys. **28**, 819 (1974)
86. R.A. Evarestov, V.P. Smirnov, J. Phys.: Condens. Matter **9**, 3023 (1997)
87. R.A. Evarestov, V.P. Smirnov, phys. stat. sol. (b) **119**, 9 (1983)
88. D. J. Chadi, M.L. Cohen, Phys. Rev. B **8**, 5747 (1973)
89. J. Moreno, J.M. Soler, Phys. Rev. B **46**, 13891 (1992)
90. H.J. Monkhorst, J.D. Pack, Phys. Rev. B **13**, 5188 (1976)
91. R.A. Evarestov, V.P. Smirnov, Phys. Rev. B **70**, 233101 (2004)
92. A. Baldereschi, Phys. Rev. B **7**, 5212 (1973)
93. D. Vanderbilt, Phys. Rev. B **41**, 7892 (1990)
94. M. Causa, R. Dovesi, C. Roetti, Phys. Rev. B **43**, 11937 (1991)
95. R.A. Evarestov, V.A. Lovchikov, I.I. Tupitsin, phys. stat. sol. (b) **117**, 417 (1983)
96. K.B. Wiberg, Tetrahedron **24**, 1083 (1968)
97. V.A. Veryazov, A.V. Leko, R.A. Evarestov Phys. Solid State **41**, 1286 (1999)
98. R.A. Evarestov, I.I. Tupitsyn, Russ. J. Phys. Chem. **74**, S363 (2000)
99. C. Pisani, E. Apra, M. Causa, Int. J. Quantum Chem. **38**, 419 (1990)
100. T. Bredow, R.A. Evarestov, K. Jug, phys. stat. sol. (b) **222**, 495 (2000)
101. V. Fock, M. Vesselow, M. Petrashen, Zh. Exsp. Theor. Fiz. **10**, 723 (1940)

102. C.J. Cramer, *Essentials of Computational Chemistry*, 2nd edn. (Wiley, New York, 2004).
103. M.J. Wong, L. Radom, J. Phys. Chem. **99**, 8582 (1995)
104. C. Moller, M.S. Plesett, Phys.Rev. **46**, 618 (1934)
105. Per-Olov Löwdin, Int. J. Quantum Chem. **55**, 77 (1995)
106. P. Knowles, M. Schütz, H.-J. Werner, in *Modern Methods and Algorithms of Quantum Chemistry*, Proceedings, 2nd edn. ed. by J. Grotendorst, John von Neumann Institute for Computing, Julich, NIC Series, **3**, 97 (2000)
107. Gaussian 03, Revision C.02, M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, J.A. Montgomery Jr., T. Vreven, K.N. Kudin, J.C. Burant, J.M. Millam, S.S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G.A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J.E. Knox, H.P. Hratchian, J.B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, P.Y. Ayala, K. Morokuma, G.A. Voth, P. Salvador, J.J. Dannenberg, V.G. Zakrzewski, S. Dapprich, A.D. Daniels, M.C. Strain, O. Farkas, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J.V. Ortiz, Q. Cui, A.G. Baboul, S. Clifford, J. Cioslowski, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, C. Gonzalez, and J.A. Pople, Gaussian, Inc., Wallingford CT, 2004, http://www.gaussian.com/citation.htm
108. http://www.eecs.harvard.edu/ mdw/proj/old/jaguar/release.html
109. C. Pisani, M. Busso, G. Capecchi, S. Casassa, R. Dovesi, L. Maschio, C. Zicovich-Wilson, M. Schutz, J. Chem. Phys. **122**, 094113 (2005)
110. P. Fulde, Adv. Phys. **51**, 909 (2002)
111. H. Stoll, Chem. Phys. Lett. **191**, 548 (1992)
112. A. Shukla, M. Dolg, P. Fulde, H. Stoll, Phys. Rev. B **60**, 5211 (1999)
113. B. Paulus, Chem. Phys. Lett. **371**, 7 (2003)
114. P.Fulde, H. Stoll, Found. Physics **30**, 2049 (2000)
115. K.N. Kudin, G.E. Scuseria, J. Chem. Phys. **113**, 7779 (2000)
116. http://www.molpro.net
117. http://www.theochem.unito.it/lcc2004/cryscor.pdf
118. B.O. Roos, Acc. Chem. Res. **32**, 137 (1999)
119. http://www.emsl.pnl.gov/docs/nwchem/
120. J. Cizek, J. Chem. Phys. **45**, 4256 (1966)
121. T.D. Crawford, J. Stanton, Int. J. Quantum Chem. **70**, 601 (1998)
122. K. Raghavachari, G.W. Trucks, J.A. Pople, M. Head-Gordon, Chem. Phys. Lett. **157**, 479 (1989)
123. K.L. Bak, A. Halkier, P. Jorgensen, J. Olsen, T. Helgaker, W. Klopper, J. Mol. Structure (Theochem) **567–568**, 375 (2001)
124. K. Hald, A. Halkier, P. Jorgensen, S. Horiani, S. Hättig, L. Helgaker, J. Chem. Phys. **118**, 2985 (2003)
125. M. Kallay, J. Gauss, J. Chem. Phys. **120**, 6841 (2004)
126. Y. He, D. Cremer, Mol. Phys. **98**, 1415 (2000)
127. M.S. Lee, P.E. Masien, M. Head-Gordon, J. Chem. Phys. **112**, 3592 (2000)
128. C. Hampel, H.-J. Werner, J. Chem. Phys. **104**, 6286 (1996)
129. P.Y. Ayala, G.E. Scuseria, J. Chem. Phys. **110**3660 (1999)
130. P. Pulay, S. Sacho, Theor. Chim. Acta **69**, 357 (1986)
131. M. Schütz, G. Hetzer, H-J. Werner, J. Chem. Phys. **111**, 5691 (1999)
132. P. Knowles, M. Schutz, H-J. Werner, in *Modern Methods and Algorithms of Quantum Chemistry*, Proceedings, 2nd edn., ed. by J. Grotendorst, John von Neumann Institute for Computing, Jeulich, NIC Series, **3**, 97 (2000).

133. M.Schütz, J. Chem. Phys. **114**, 661 (2001)
134. M.Schütz, J. Chem. Phys. **116**, 8772 (2002)
135. S.Goedecker, G.Scuseria, Comput. Sci. Eng., **5**(4), 14 (2003)
136. S. Saebo, P. Pulay, J. Chem. Phys. **86**, 914 (1987)
137. M. Haser, J. Almlöf, J. Chem. Phys. **96**, 489 (1992)
138. P. Constans, G.E. Scuseria, Collect. Czech. Chem. Commun. **68**, 357 (2003)
139. M. Schütz, H-J. Werner, R. Lindh, F.R. Manby, J. Chem. Phys. **121**, 737 (2004)
140. A. Hesselmann, G. Jansen, M.Schütz J. Chem. Phys. **122**, 014103 (2005)
141. M. Schütz, G. Rauhut, H.-J. Werner, J. Phys. Chem. A **102**, 5997 (1998)
142. M. Schütz, Phys. Chem. Chem. Phys. **4**, 3941 (2002)
143. G.E. Scuseria, P.Y. Ayala, J. Chem. Phys. **111**, 8330 (1999)
144. J.W. Boughton, P.Pulay, J. Comput. Chem. **14**, 736 (1993)
145. G. Hetzer, P. Pulay, H-J. Werner, Chem. Phys. Lett. **290**, 143 (1998)
146. H-J. Werner, F.R. Manby, P.J. Knowles, J. Chem. Phys. **118**, 8149 (2003)
147. M.Shütz, F.R. Manby, Phys. Chem. Chem. Phys. **5**, 3349 (2003)
148. F. Weigend, M. Häser, Theor. Chim. Acta **97**, 331 (1997)
149. M. Schütz, J. Chem. Phys. **113**, 9986 (2000)
150. W. Heitler, F. London, Z. Phys. **44**, 455 (1927)
151. *Strong Coulomb Correlations in Electronic Structure Calculations. Beyond the Local Density Approximation*, ed. by Vladimir I.Anisimov (Gordon and Breach Sci. Publ., Amsterdam, 2000)
152. J.P. Perdew, A. Zunger, Phys. Rev. B **23**, 5048 (1991)
153. V.I. Anisimov, J. Zaanen, O.K. Andersen, Phys. Rev. B **44**, 943 (1991)
154. C. Pisani, J. Molec. Structure (Theochem) **621**, 141 (2003)
155. C.M. Zicovich-Wilson, R. Dovesi, Chem. Phys. Lett. bf 277, 227 (1997)
156. http://www.theochem.unito.it/lcc2004/
157. D.E. Usvyat, M. Schütz, Theor. Chem. Acc. **114**, 276 (2005)
158. A. Shukla, M. Dolg, H. Stoll, P. Fulde, Phys. Rev. B **57**, 1471 (1998)
159. B. Paulus, P. Fulde, H. Stoll, Phys.Rev B **51**, 10572 (1995)
160. B. Paulus, Physics Reports **428**, 1 (2006)
161. W.Kutzelnigg, in: *Methods of Electronic Structure Theory*, ed. by H.F. SchaeferIII (Plenum, New York, 1977), pp.129
162. H. Stoll, B. Paulus, P. Fulde, J. Chem. Phys. **123**, 144108 (2005)
163. B. Paulus, P. Fulde, H. Stoll, Phys. Rev. B **54**, 2556 (1996)
164. M. Albrecht, B. Paulus, H. Stoll, Phys. Rev. B **56**, 7339 (1997)
165. K. Doll, M. Dolg, P. Fulde, H. Stoll, Phys. Rev. B **52**, 4842 (1995)
166. K. Doll, M. Dolg, H. Stoll, Phys. Rev. B **54**, 13529 (1996)
167. K. Doll, M. Dolg, P. Fulde, H. Stoll, Phys. Rev. B **55**, 10282 (1997)
168. K. Doll, H. Stoll, Phys. Rev. B **57**, 4327 (1998)
169. K. Rosciszewski, K. Doll, B. Paulus, P. Fulde, H. Stoll, Phys. Rev. B **57**, 14667 (1998)
170. K. Rosciszewski, B. Paulus, P. Fulde, H. Stoll, Phys. Rev. B **60**, 7905 (1999)
171. K. Rosciszewski, B. Paulus, P. Fulde, H. Stoll, Phys. Rev. B **62**, 5482 (2000)
172. B. Paulus, K. Rosciszewski, N.Gaston, P. Schwerdtfeger, H. Stoll, Phys. Rev. B **70**, 165106 (2004)
173. N. Gaston, B. Paulus, K. Rosciszewski, P. Schwerdtfeger, H. Stoll, Phys. Rev. B **74**, 094102 (2006)
174. S. Kalvoda, M. Dolg, H.-J. Flad, P. Fulde, H. Stoll, Phys. Rev. B **57**, 2127 (1998)
175. E. Voloshina, B. Paulus, Theor. Chem. Acc. **114**, 259 (2005)
176. J. Gräfenstein, H. Stoll, P. Fulde, Chem. Phys. Lett. **215**, 611 (1993)
177. J. Gräfenstein, H. Stoll, P. Fulde, Phys. Rev. B **55**, 13588 (1997)
178. M. Albrecht, P. Reinhardt, J.-P. Malrieu, Theor. Chem. Acc. **100**, 241 (1998)
179. A. Abdurahman, M. Albrecht, A. Shukla, M. Dolg, J. Chem. Phys. **110**, 8819 (1999)

180. M. Albrecht, P. Fulde, H. Stoll, Chem. Phys. Lett. **319**, 355 (2000)
181. A. Shukla, M. Dolg, P. Fulde, H. Stoll, Phys. Rev. B **57**, 1471 (1998)
182. R. Orlando, R. Dovesi, C. Roetti, V.R. Saunders, J. Phys: Condens. Matter **2**, 7769 (1990)
183. P. Fulde, Theor. Chem. Acc. **114**, 255 (2005)
184. J.Q. Sun, R.J. Bartlett, J. Chem. Phys. **104**, 8553 (1996)
185. P.Y. Ayala, K.N. Kudin, G.E. Scuseria, J. Chem. Phys. **115**, 9698 (2001)
186. J. Almlöf, Chem. Phys. Lett. **181**, 319 (1991)
187. M. Haser, Theor. Chim. Acta **87**, 147 (1993)
188. R. Pino, G.E. Scuseria, J. Chem. Phys. **121**, 2553 (2004)
189. P.Y. Ayala, G.E. Scuseria, Chem. Phys. Lett. **322**, 213 (2000)
190. A. Zunger, A. Katzir, A. Halperin, Phys. Rev. B **13**, 5560 (1976)
191. K. Kobayashi, T. Sano, Y. I'Haya, Chem. Phys. Lett. **219**, 53 (1994)
192. C. Pisani, G. Capecchi, S. Casassa, L. Maschio, Mol. Phys. **103**, 2527 (2005)
193. W. Boughton, P. Pulay, J. Comput. Chem. **14**, 736 (1993)
194. W. Kohn, Phys. Rev. **115**, 809 (1959)
195. P.W. Anderson, Phys. Rev. Lett. **21**, 13 (1968)
196. P. Zeiner, R. Dirl, B.L. Davies, Phys. Rev. B **58**, 7681 (1998)
197. L. He, D. Vanderbilt, Phys. Rev. Lett. **86**, 5341 (2001)
198. R.A. Evarestov, D.E. Usvyat, V.P. Smirnov, Phys. Solid State **45**, 2072 (2003)
199. S. Lui, J.M. Perez-Jorda, W. Yang, J. Chem. Phys. **112**, 1634 (2000)
200. H. Feng, J. Bian, L. Li, W. Yang, J. Chem. Phys. **120**, 9458 (2004)
201. S. Casassa, C.M. Zicovich-Wilson, C. Pisani, Theor. Chem. Acc. **116**, 726 (2006)
202. C.M. Zicovich-Wilson, R. Dovesi, Int. J. Quantum Chem. **67**, 299(1998)
203. C.M. Zicovich-Wilson, R. Dovesi, V.R. Saunders, J. Chem. Phys. **115**, 9708 (2001)
204. R. Hoffmann, J. Chem. Phys. **39**, 1397 (1963)
205. J.A. Pople, D.L. Beveridge, *Approximate Molecular Orbital Theory* (McGraw-Hill, N.Y., 1970)
206. E.B. Moore, C.M. Carlson, Phys. Rev. B **4**, 2063 (1971)
207. R. Dovesi, C. Pisani, F.Ricca, C. Roetti, Chem. Phys. Lett. **39**, 103 (1976)
208. A.R. Leach, *Molecular Modelling:Principles and Applications*, 2nd edn. (Pearson Education EMA, 2001)
209. R. Canadine, I. Hiller, J. Chem. Phys. **50**, 2985 (1969)
210. J.C. Slater, Phys. Rev. **36**, 57 (1930)
211. J. Hinze, H.H. Jaffe, J. Am. Chem. Soc. **84**, 540 (1962)
212. L.C. Cusachs, J.W. Reinolds, D. Barnard, J. Chem. Phys. **44**, 835 (1966)
213. M. Wolfsberg, L.J. Helmholz, J. Chem. Phys. **20**, 837 (1952)
214. M. Nishida, Phys. Rev. B **58**, 7103 (1998)
215. J.R. Chelikowsky, M.L. Cohen, Phys. Rev. B **10**, 5095 (1974)
216. J. Cerda, F. Soria, Phys. Rev. B **61**, 7965 (2000)
217. A. Herman, Modeling Simul. Mater. Sci. Eng. **12**, 21 (2004)
218. W. Koch, B. Frey, J.F.S. Ruiz, T. Scior, Z. Naturforsch. **58a**, 756 (2003)
219. K. Ruedenberg, J. Chem. Phys. **19**, 1433 (1951)
220. R.S. Mulliken, J. Chim. Phys. **46**, 500, 521 (1949)
221. R. Fenske, K. Caulton, D. Radtke, C. Sweeney, Inorg. Chem. **5**, 951 (1966)
222. R.A. Evarestov, A.N. Ermoshkin, phys. stat. sol. (b) **86**, 47 (1978)
223. W. Koch, B. Frey, J.F.S. Ruiz, T. Scior, Z. Naturforsch. **58a**, 785 (2003)
224. A.N. Ermoshkin, E.A. Kotomin, A.L. Shluger, J. Phys. C: Solid State Phys. **15**, 847 (1982)
225. P.O. Löwdin, J. Chem. Phys. **18**, 365 (1950)
226. A.N. Ermoshkin, E.A. Kotomin, R.A. Evarestov, phys. stat. sol. (b) **72**, 787 (1975)

227. G.A. Bordovskii, M.L. Gordeev, A.N. Ermoshkin, R.A. Evarestov, phys. stat. sol. (b) **111**, K123 (1982)
228. R.A. Evarestov, A.N. Ermoshkin, V.A. Lovchikov, phys. stat. sol. (b) **99**, 387 (1980)
229. A.N. Ermoshkin, R.A. Evarestov, Optica i Spectroskopija **35**, 786 (1973)
230. A.N. Ermoshkin, R.A. Evarestov, phys. stat. sol. (b) **66**, 687 (1974)
231. A.N. Ermoshkin, R.A. Evarestov, E.A. Kotomin, phys. stat. sol. (b) **73**, 81 (1976)
232. R.A. Evarestov, A.N. Ermoshkin, Optica i Spectroskopija **40**, 610 (1976)
233. R.A. Evarestov, A.N. Ermoshkin, E.A. Kotomin, phys. stat. sol. (b) **73**, 483 (1976)
234. A.N. Ermoshkin, E.A. Kotomin, R.A. Evarestov, phys. stat. sol. (b) **103**, 581 (1981)
235. T. Bredow, K. Jug, Theor. Chem. Acc. **113**, 1 (2005)
236. J.A. Pople, D.P. Santry, G.A. Segal, J. Chem. Phys. **43**, S129 (1965)
237. R. Pariser, G.R. Parr, J. Chem. Phys. **21**, 466, 767 (1953)
238. N. Mataga, K. Nishimoto, Z. Phys. Chem. **13**, 140 (1957)
239. K. Ohno, Adv. Quantum Chem. **3**, 240 (1967)
240. M.G. Veselov, M.M. Mestechkin, Theor. Exp. Chem. **6**, 471 (1973)
241. J.A. Pople, D.L. Beveridge, P.A. Dobosh, J. Chem. Phys. **47**, 2026 (1967)
242. Da Motta Neto, M.C. Zerner Int. J. Quantum Chem. **81**, 187 (2001)
243. J.E. Ridley, M.C. Zerner, Theor. Chim. Acta **32**, 111 (1973)
244. M. Kotzian, N. Rosch, M.C. Zerner, Theor. Chim. Acta **81**, 201 (1992)
245. R.C. Bingham, M.J.S. Dewar, D.H. Lo, J. Am. Chem. Soc. **97**, 1285, 1307 (1975)
246. M.J.S. Dewar, E.G. Zoebisch, E.F. Healey, J.J.P. Stewart, J. Am. Chem. Soc. **107**, 3902 (1985)
247. W.Thiel, J. Am. Chem. Soc. **103**, 1413, 1421 (1981)
248. J.J.P. Stewart, J. Comput. Chem. **10**, 209 (1989)
249. D.N. Nanda, K. Jug, Theor. Chim. Acta **57**, 95 (1980)
250. K. Jug, R.Iffert, J. Schulz, Int. J. Quantum Chem. **32**, 265 (1987)
251. J. Li, P. Correa de Mello, K. Jug, J. Comput. Chem. **13**, 85 (1992)
252. M.C. Zerner, Mol. Phys. **23**, 963 (1972)
253. B. Ahlswede, K. Jug, J. Comput. Chem. **20**, 563 (1999)
254. B. Ahlswede, K. Jug, J. Comput. Chem. **20**, 572 (1999)
255. K. Jug, G. Geudtner, T. Homann, J. Comput. Chem. **21**, 974 (2000)
256. T. Bredow, G. Geudtner, K. Jug, J. Comput. Chem. **22**, 861 (2001)
257. T. Bredow, K. Jug, in *Encyclopedia of Computational Chemistry (online edition)*, eds. P. Schleyer, N.L. Allinger, T. Clark, J. Gasteiger, P.A. Kollman, H.F. Schaefer III, P.R. Schreiner (Wiley, Chicester, 2004)
258. J. Schultz, R. Iffert, K. Jug, Int. J. Quantum Chem. **27**, 461 (1985)
259. B. Voigt, Theor. Chim. Acta **31**, 289 (1973)
260. C. Kollmar, M.C. Böhm, Theor. Chim. Acta **92**, 13 (1995)
261. C. Kollmar, Chem. Phys. Lett. **269**, 215 (1997)
262. C. Kollmar, B.A. Hess, Mol. Phys. **100**, 1945 (2002)
263. H. Fujita, A. Imamura, J. Chem. Phys. **53**, 4555 (1970)
264. S. O'Shea, D.P. Santry, J. Chem. Phys. **54**, 2667 (1971)
265. K. Mororuma, J. Chem. Phys. **54**, 962 (1971)
266. B.J. McAloon, P.G. Perkins, J. Chem. Soc. Faraday Trans.II **68**, 1121, 1833 (1972)
267. D.L. Beveridge, I. Jano, J. Ladik, J. Chem. Phys. **56**, 4744 (1972)
268. M.C. Böhm, Theor. Chim. Acta **62**, 351, 373 (1983)
269. M.J.S. Dewar, K.M. Merz Jr, Organometallics **5**, 1494 (1986)
270. J.J.P. Stewart, New Polym. Mater. **1**, 53 (1987)
271. J. Chandrasekhar, P.K. Das, J. Phys. Chem. B **96**, 679 (1992)
272. L.Y.A. Davila, M.J. Caldas, J. Comput. Chem. **23**, 1135 (2002)
273. F. Ricca, J. Phys. (Paris) **38, Suppl.C-4**, 173 (1977)
274. R. Dovesi, C. Pisani, F. Ricca, C. Roetti, Surf. Sci. **75**, 316 (1978)

275. R. Dovesi, C. Pisani, F. Ricca, C. Roetti, J. Chem. Phys. **65**, 3075, 4116 (1976)
276. R.A. Evarestov, V.A. Lovchikov, phys. stat. sol. (b) **79**, 743 (1977)
277. A.H. Harker, F.P. Larkins, J. Phys. C: Solid State Phys. **12**, 2487 (1979)
278. R. Dovesi, C. Pisani, C. Roetti, Surf. Sci. **103**, 482 (1981)
279. P.G. Perkins, A.K. Marwaha, J.J.P. Stewart, Theor. Chim. Acta **57**, 1 (1980)
280. P.V. Smith, J.E. Szymanski, J.A.D. Matthew, J. Phys.: Solid State Phys. **18**, 3157 (1985)
281. R.Ramirez, M.C. Böhm, Int. J. Quantum Chem. **34**, 47 (1988)
282. R. Dovesi, C. Pisani, C. Roetti, J.M. Ricart, F.Illas, Surf. Sci. **148**, 225 (1984)
283. B.I. Craig, P.V. Smith, Surf. Sci. **210**, 468 (1989)
284. J.D. Weibel, D. Yaron, J. Chem. Phys. **116**, 6846 (2002)
285. A.J. Bennett, B. McCarroll, R.P. Messmer, Phys. Rev. B **3**, 1397 (1971)
286. A. Zunger, J.Phys. C: Solid State Phys. **7**, 76 (1974)
287. A. Zunger, J. Chem. Phys. **62**, 1861 (1975)
288. R.P. Messmer, G.D.Watkins in *Radiation Damage and Defects in Semiconductors*, N16, p.255, Institute of Physics, London (1973)
289. A.M. Dobrotvorskii, R.A. Evarestov, phys. stat. sol. (b) **66**, 83 (1974)
290. R.A. Evarestov, M.I. Petrashen, E.M. Ledovskaya, phys. stat. sol. (b) **76**, 377 (1976)
291. *Hartree-Fock-Slater Method for Materials Science. The DV-X Alpha Method for Design and Characterization of Materials*, eds. H.Adachi, T.Mukoyama, J. Kawai, in Springer Series in Materials Science, vol. **84**, (Spinger, Berlin, Heidelberg, New York, 2006)
292. U.Lindefeldt, J. Phys. C: Solid State Phys. **11**, 85 (1978)
293. P. Deak, L. Snyder, Phys. Rev. B **36**, 9619 (1987)
294. P. Deak, phys. stat. sol. (b) **217**, 9 (2000)
295. R.A. Evarestov, M.I. Petrashen, E.M. Ledovskaya, phys. stat. sol. (b) **68**, 453 (1975)
296. V.A. Koptsik, R.A. Evarestov, Kristallographia **25**, 5 (1980)
297. R.A. Evarestov, A.V. Leko, V.P. Smirnov, phys. stat. sol. (b) **128**, 275 (1985)
298. P.G. Perkins, J.J.P. Stewart, J. Chem. Soc. Faraday II **76**, 520, 534 (1980)
299. J.J.P. Stewart, J. Comput. Chem. **19**, 168 (1998)
300. R.A. Evarestov, V.A. Lovchikov, phys. stat. sol. (b) **93**, 469 (1979)
301. T. Bredow, G.Geudtner, K. Jug, Int. J. Quantum Chem. **22**, 89 (2001)
302. F. Janetzko, T. Bredow, K. Jug, J. Chem. Phys. **116**, 8994 (2002)
303. P. Deak, Phys. Lett. A **83**, 39 (1981)
304. A.L. Shluger, E.A. Kotomin, phys. stat. sol. (b) **108**, 673 (1981)
305. R.A. Evarestov, V.A. Veryazov, phys. stat. sol. (b) **157**, 281 (1990)
306. R.A. Evarestov, V.A. Veryazov, Rev. Solid State Sci. **5**, 415 (1991)
307. J. Noga, P. Banacky, S. Biskupic, R. Boca, P. Pelikan, M. Svrcek, A. Zajac, Int. J. Quantum Chem. **20**, 253 (1999)
308. P. Pelikan, J. Noga, S. Biskupic, J. Solid State Chem. **174**, 233 (2003)
309. E. Stefanovich, E. Shidlovskaya, A. Schluger, phys. stat. sol. (b) **160**, 529 (1990)
310. S.S. Moliver, Phys. Solid State **42**, 673 (2000)
311. A.O. Litinskii, I.P. Zakharov, J. Struct. Chem. **27**, 517 (1986)
312. J.J.P. Stewart, J. Molec. Struct. (Theochem) **556**, 59 (2000)
313. A. Schluger, Theor. Chim. Acta **66**, 355 (1985)
314. A.H. Harker, F.P. Larkins, J. Phys. C: Solid State Phys. **12**, 2509 (1979)
315. E.A. Kotomin, A.L. Schluger, phys. stat. sol. (b) **109**, 75 (1982)
316. A.H. Harker, F.P. Larkins, J. Phys. C: Solid State Phys. **12**, 2497 (1979)
317. P.V. Smith, J.E. Szymanski, J.A.D. Matthew, phys. stat. sol. (b) **136**, 261 (1986)
318. R.A. Evarestov, V.A. Veryazov, phys. stat. sol. (b) **158**, 201 (1990)
319. A. Porreda, V.A. Lovchikov, K. Jug in *NATO ASI Series B* Cluster Models for Surface and Bulk Phenomena, eds. G. Pacchioni, P.S. Bagus, F. Parmigiani, Plenum New York, 1992, **283**, p.641

320. K. Jug, T. Bredow, J. Comput. Chem. **25**, 1551 (2004)
321. K. Jug, T. Bredow in *Methods and Techniques in Computational Chemistry, METECC-95*, ed. E. Clementi, p. 89, STEF, Calgari (1995)
322. R. Dovesi, V.R. Saunders, C. Roetti, N.M. Harrison, R.Orlando, E. Apra, Crystal95 User's Manual, Universita di Torino, Torino (1996)
323. B. Silvi, N. Fouranti, R. Nada, C.R. Catlow, J. Phys. Chem. Solids **52**, 1005 (1991)
324. C. Pisani, R. Dovesi, C. Roetti, *Hartree–Fock ab-initio Treatment of Crystalline Systems*, Lecture Notes in Chemistry **48**, Springer-Verlag, Berlin (1988)
325. L.H. Thomas, Proc. Camb. Philos. Soc. **23**, 542 (1927)
326. E. Fermi, Z. Phys. **48**, 73 (1928)
327. J.C. Slater, Phys. Rev. **91**, 528 (1953)
328. P. Hohenberg, W. Kohn, Phys. Rev. **136**, B864 (1964)
329. N.C. Handy, Molec. Phys. **102**, 2399 (2004)
330. K. Capelle, *A Birds-eye View of Density Functional Theory*, http://arXiv.org/archive/cond-mat/0211443v4
331. W. Kohn, Rev. Mod. Phys. **71**, 1253 (1998)
332. W. Kohn, L.J. Sham, Phys. Rev. **140**, A1133 (1965)
333. R.M. Dreizler, E.K.U. Gross, *Density Functional Theory* (Springer, Berlin, 1990).
334. N.H. March, *Electron Density Theory of Atoms and Molecules* (Academic Press, London, 1992).
335. H. Eschrig, *The Fundamentals of Density Functional Theory* (Teubner, Leipzig, 1996).
336. *Density Functional Theory: Recent Progress and New Directions*, eds. J.F. Dobson, G. Vignale, M.P. Das (Plenum, New York, 1998)
337. W. Koch, M.C. Holthausen, *A Chemist's Guide to Density Functional Theory*, 2nd edn. (John Wiley, New York, 2002).
338. R.O. Jones, O. Gunnarsson, Rev. Mod. Phys. **61**, 689 (1989)
339. R. Neumann, Molec. Phys. **87**, 1(1996)
340. J.P. Perdew, S. Kurth, Lecture Notes in Phys. **620**, 1 (2003)
341. K. Burke, J. Werschnik, E.K.U. Gross, J. Chem. Phys. **123**, 062206 (2005)
342. I.G. Kaplan, *Intermolecular Interactions. Physical Picture, Computational Methods and Model Potentials*, (Wiley, 2006).
343. K. Capelle, V.L. Libero, Int. J. Quantum Chem. **105**, 679 (2005)
344. http://www.uam.es/departamentos/ciencias/fismateriac/siesta/
345. http:///www.scm.com/Doc/Doc2006.01
346. J.C. Slater, Phys. Rev. **81**, 385 (1951)
347. P.A.M. Dirac, Proc. Camb. Philos. Soc. **26**, 376 (1930)
348. U. von Barth, L. Hedin, J. Phys. C: Condens. Matter **5**, 1629 (1972)
349. O. Gunnarsson, B.I. Lundqvist, Phys. Rev. B **13**, 4274 (1976)
350. D.M. Ceperley, B.J. Alder, Phys. Rev. Lett. **45**, 566 (1980)
351. S.J. Vosko, L. Wilk, M. Nussair, Can. J. Phys. **1980**, 1200 (1980)
352. J.P. Perdew, A. Zunger, Phys. Rev. B **23**, 5048 (1981)
353. J.P. Perdew, Y. Wang, Phys. Rev. B **40**, 3389 (1989)
354. J.P. Perdew, A. Zunger, Phys. Rev. B **45**, 13244 (1992)
355. J.P. Perdew, A. Zunger, Phys. Rev. B **33**, 8800 (1986)
356. J.P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996)
357. J.P. Perdew, A. Ruzsinszky, J. Tao, V.N. Staroverov, G.E. Scuseria, G.I. Csonka, J. Chem. Phys. **123**, 062201 (2005)
358. A.D. Becke, Phys. Rev. A **38**, 3098 (1988)
359. C. Lee, W. Wang, R.G. Parr, Phys. Rev. B **37**, 785 (1988)
360. J. Tao, J.P. Perdew, V.N. Staroverov, G.E. Scuseria, Phys. Rev. Lett. **91**, 146401 (2003)
361. Xin Xu, W.A. Goddard III, J. Chem. Phys. **121**, 4068 (2004)
362. J. Tao, J.P. Perdew, V.N. Staroverov, G.E. Scuseria, Phys. Rev. B **69**, 075102 (2004)

363. J.P. Perdew, S. Kurth, A. Zupan, P. Blaha, Phys. Rev. Lett. **82**, 2544 (1999)
364. J.P. Perdew, K. Burke, Y. Wang, Phys. Rev. B **54**, 16533 (1996)
365. P. Ziesche, S. Kurth, J.P. Perdew, Comput. Mater. Sci. **11**, 122 (1998)
366. E.H. Lieb, S. Oxford, Int. J. Quantum Chem. **19**, 427 (1981)
367. E.J. Baerends, O.V. Gritsenko, J. Chem. Phys. **123**, 062202 (2005)
368. M. Gruning, O.V. Gritsenko, E.J. Baerends, J. Chem. Phys. **118**, 7183 (2003)
369. E.J. Baerends, Phys. Rev. Lett. **87**, 133004 (2001)
370. M.A. Buijse, E.J. Baerends, Molec. Phys. **100**, 401 (2002)
371. F. Cora, M. Alfredsson, G. Mallia, D. Midlemiss, W.C. Mackrodt, R. Dovesi, R. Orlando, Struct. and Bond. **113**, 171 (2004)
372. A.D. Becke, J. Chem. Phys. **112**, 4020 (2000)
373. A.D. Becke, J. Chem. Phys. **98**, 1372, 5468 (1993)
374. O.V. Gritsenko, P.R. T.Schipper, E.J. Baerends, Int. J. Quantum Chem. Symp. **30**, 1375 (1996)
375. J.P. Perdew, M. Ernzerhof, K. Burke, J. Chem. Phys. **105**, 9982 (1996)
376. J.E. Jaffe, A.C. Hess, J. Chem. Phys. **105**, 10983 (1996)
377. M.C. Payne, M.P. Teller, D.C. Allan, J.A. Arias, J.D.Joannopoulos, Rev. Mod. Phys. **64**, 1045 (1992)
378. http://www.wien2k.at
379. K.N. Kudin, G.E. Scuseria, Phys. Rev. B **61**, 16440 (2000)
380. V.N. Staroverov, G.E. Scuseria, J. Tao, J.P. Perdew, Phys. Rev. B **69**, 075102 (2004)
381. L. Greengard, V. Rokhlin, J. Comput. Phys. **73**, 325 (1987)
382. K.N. Kudin, G.E. Scuseria, Chem. Phys. Lett. **289**, 611 (1998)
383. E. Artacho, D. Sanchez-Portal, P. Ordejon, A. Garcia, J.M. Soler, phys. stat. sol. (b) **215**, 809 (1999)
384. P. Ordejon, E. Artacho, J.M. Soler, Phys. Rev. B **53**, R10441 (1996)
385. J.R. Chelikowsky, S.G. Loucie, Phys. Rev. B **29**, 3470 (1987)
386. G. Velde, E.J. Baerends, Phys. Rev. B **44**, 7888 (1991)
387. P.J. Feibelman, Phys. Rev. B **44**, 3916 (1991)
388. G. Seifert, D. Porezug, Th. Frauenheim, Int. J. Quantum Chem. **58**, 185 (1996)
389. M. Towler, A. Zupan, M. Causa, Comput. Phys. Commun. **98**, 181 (1996)
390. A. Lichanot, M. Merawa, M. Causa, Chem. Phys. Lett. **246**, 263 (1995)
391. A. Zupan, M. Causa, Int. J. Quantum Chem. **56**, 337 (1995)
392. A. Savin, Int. J. Quantum Chem. **S22**, 457 (1988)
393. A.D. Becke, J. Chem. Phys. **96**, 2155 (1992)
394. M. Causa, Lecture Notes in Chem. **48**, 91 (1996)
395. F. Figueirido, R.M. Levy, R. Zhou, B. Berne, J. Chem. Phys. **106**, 9835 (1997)
396. M. Challacombe, C. White, M. Head-Gordon, J. Chem. Phys. **107**, 1013 (1997)
397. K.N. Kudin, G.E. Scuseria, J. Chem. Phys. **121**, 2886 (2004)
398. K.N. Kudin, G.E. Scuseria, Phys. Rev. B **61**, 5141 (2000)
399. D.L. Strout, G.E. Scuseria, J. Chem. Phys. **102**, 8448 (1995)
400. J.M. Soler, E. Artacho, J.D. Gale, A. Garcia, J. Junquera, P. Ordejon, D. Sanchez-Portal, J. Phys.: Condens. Matter **14**, 2745 (2002)
401. E. Anglada, J.M. Soler, J.Junquera, E. Artacho, Phys. Rev. B **66**, 205101 (2002)
402. M.C. Strain, G.E. Scuseria, M.J. Frisch, Science **271**, 51 (1996)
403. J.C. Burant, M.C. Strain, G.E. Scuseria, M.J. Frisch, Chem. Phys. Lett. **258**, 45 (1998)
404. P. Pulay, J. Comput. Chem. **3**, 556 (1982)
405. R.E. Stratmann, G.E. Scuseria, M.J. Frisch, 257 **257**, 213 (1996)
406. http://www.gaussian.com/g people/gus.htm
407. C. Adamo, V. Barone, J. Chem. Phys. **110**, 6158 (1999)
408. J. Heyd, G.E. Scuseria, M. Ernzerhof, J. Chem. Phys. **118**, 8207 (2003)
409. J. Heyd, G.E. Scuseria, J. Chem. Phys. **120**, 7274 (2004)

410. W. Kohn, Int. J. Quantum Chem. **56**, 229 (1995)
411. J.P. Perdew, M. Ernzerhof, K. Burke, J. Chem. Phys. **105**, 9982 (1996)
412. M. Ernzerhof, G.E. Scuseria, J. Chem. Phys. **110**, 5029 (1999)
413. J.C. Burant, G.E. Scuseria, M.J. Frisch, J. Chem. Phys. **105**, 8969 (1996)
414. E. Schwegler, M. Challacombe, J. Chem. Phys. **105**, 2726 (1996)
415. C. Ochsenfeld, C.A. White, M. Head-Gordon, J. Chem. Phys. **109**, 1163 (1998)
416. M.W. Gill, J.A. Pople, Int. J. Quantum Chem. **40**, 753 (1991)
417. M. Ernzerhof, J.P. Perdew, J. Chem. Phys. **109**, 3313 (1998)
418. GAUSSIAN Development Version, Revision B.07, M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, J.A. Montgomery Jr., T. Vreven, K.N. Kudin, J.C. Burant, J.M. Millam, S.S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G.A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J.E. Knox, H.P. Hratchian, J.B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, P.Y. Ayala, K. Morokuma, G.A. Voth, P. Salvador, J.J. Dannenberg, V.G. Zakrzewski, S. Dapprich, A.D. Daniels, M.C. Strain, O. Farkas, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J.V. Ortiz, Q. Cui, A.G. Baboul, S. Clifford, J. Cioslowski, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, C. Gonzalez, and J.A. Pople, Gaussian Inc., Pittsburg, PA, 2003
419. J. Heyd, J.E. Peralta, G.E. Scuseria, R.L. Martin, J. Chem. Phys. **123**, 174101 (2005)
420. J. Uddin, G.E. Scuseria, Phys. Rev. B **72**, 035101 (2005)
421. J. Uddin, J.E. Peralta, G.E. Scuseria, Phys. Rev. B **71**, 155112 (2005)
422. I.D. Prodan, G.E. Scuseria, J.A. Sordo, K.N. Kudin, R.L. Martin, J. Chem. Phys. **123**, 014703 (2005)
423. V. Barone, J.E. Peralta, J. Uddin, G.E. Scuseria, J. Chem. Phys. **124**, 024709 (2006)
424. I.D. Prodan, G.E. Scuseria, R.L. Martin, Phys. Rev. B **73**, 045104 (2006)
425. J. Paier, R. Hirschl, M. Marsman, G. Kresse, J. Chem. Phys. **122**, 234102 (2005)
426. V.R. Saunders, R. Dovesi, C. Roetti, M. Causa, N.M. Harrison, R. Orlando, C.M. Zicovich-Wilson, Crystal98 User's Manual, University of Torino, Torino (1998)
427. M.S. Hybertsen, S.G. Louie, Phys. Rev. Lett. **55**, 1418 (1985)
428. M.C. Foulkes, L. Mitas, R. Needs, G. Rajagopal, Rev. Mod. Phys. **73**, 33 (2001)
429. T. Bredow, A.R. Gerson, Phys. Rev. B **61**, 5194 (2000)
430. I. Moreira, F. Illas, R.L. Martin, Phys. Rev. B **65**, 155102 (2002)
431. W.C. Mackrodt, D.S. Middlemiss, T.G. Owens, Phys. Rev. B **69**, 115119 (2004)
432. F. Illas, R.L. Martin, J. Chem. Phys. **108**, 2519 (1998)
433. J. Muscat, A.Wander, N.M. Harrison, Chem. Phys. Lett. **342**, 397 (2001)
434. W.G. Aulbur, L. Johnsson, J.W. Wilkins, Solid State Phys. **54**, 1 (2000)
435. F. Aryasetiawan, in Strong Coulomb Correlations in Electronic Structure Calculations, ed. V.I. Anisimov, p.1 (Gordon and Breach, Singapore, 2000)
436. J.P. Perdew, S. Kurth, A. Zupan, P. Blaha, Phys. Rev. Lett. **82**, 544 (1999)
437. L. Petit, A. Svane, Z. Szotek, W.M. Temmerman, Phys. Rev. B **72**, 205118 (2005)
438. T. Fujiwara, M. Arai, Y. Ishii, in Strong Coulomb Correlations in Electronic Structure Calculations, ed. V.I. Anisimov, p.167 (Gordon and Breach, Singapore, 2000)
439. V.I. Anisimov, A.I. Lichtenstein, in Strong Coulomb Correlations in Electronic Structure Calculations, ed. V.I. Anisimov, p.97 (Gordon and Breach, Singapore, 2000)
440. V. Polo, E. Kraka, D.Cremer, Molec. Phys. **100**, 1771 (2002)
441. D.Cremer, Molec. Phys. **99**, 1899 (2001)
442. G.I. Csonka, B.J. Johnson, Theor. Chem. Acc. **99**, 158 (1998)
443. O.A. Vydrov, G.E. Scuseria, J. Chem. Phys. **121**, 8187 (2004)

444. O.A. Vydrov, G.E. Scuseria, J. Chem. Phys. **122**, 184107 (2005)
445. A. Svane, W.M. Temmerman, Z. Szotek, J. Laegsgaard, H. Winter, Int. J. Quantum Chem. **77**, 799 (2000)
446. A. Flipetti, N.A. Spaldin, Phys. Rev. B **67**, 125109 (2003)
447. M. Arai, T. Fujiwara, Phys. Rev. B **51**, 1477 (1995)
448. O.K. Anderson, Phys. Rev. B **12**, 3060 (1975)
449. M. Imada, A. Fujimori, Y. Tokura, Rev. Mod. Phys. **70**, 1040 (1998)
450. A. Rohrbach, J. Hafner, G. Kresse, J. Phys. C: Condens. Matter **15**, 979 (2003)
451. G. Kresse, J. Furthmuller, Comput. Mater. Sci. **6**, 15 (1996)
452. G. Ricardo, F. Cora, A.A. Sokol, N.H. de Leeuw, C.R.A. Catlow, Phys. Rev. B **73**, 035116 (2006)
453. S.ZN. Karazhanov, P. Ravindran, A. Kjekhus, H. Fjellvag, U. Grossner, B.G. Svensson, J. Cryst. Growth **287**, 162 (2006)
454. A.G. Eguiluz, O.D. Restrepo, B.C. Larson, J.Z. Tischler, P. Zschack, G.E. Jellison, J. Phys. Chem. Solids **66**, 2281 (2005)
455. R. Laskowskii, P. Blaha, K. Schwarz, Phys. Rev. B **67**, 075102 (2003)
456. A.L. Ivanovskii, T.I. Chupakhina, V.G. Zubkov, A.P. Tyutyunnik, V.N. Krasilnikov, G.V. Bazuev, S.V. Okatov, A.I. Lichtenstein, Phys. Lett. A **348**, 66 (2005)
457. Y. Wang, D.J. Doren, Solid State Commun. **136**, 142 (2005)
458. M. Towler, *An introductory guide to Gaussian basis sets in solid state electronic structure calculations*, http://www.crystal.unito.it/tutojan2004/tutorials/index.html
459. A.D. McLean, R.S. McLean, *Roothaan-Hartree-Fock atomic wave functions (Slater basis-set expansions for Z=55-92)*, Atomic Data and Nuclear Data Tables, **26**, 197 (1981)
460. S. Huzinaga, J. Chem. Phys. **42**, 1293 (1965)
461. M. Challacombe, J. Cioslowsky, J. Chem. Phys. **100**, 464 (1994)
462. T.H. Dunning, J. Chem. Phys. **90**, 1007 (1989)
463. http://www.emsl.pnl.gov/forms/basisform.html
464. K. Doll, N.M. Harrison, V.R. Saunders, J. Phys.: Condens. Matter **11**, 5007 (1999)
465. J. Sauer, P. Ugliengo, E. Garrone, V.R. Saunders, Chem. Rev. **94**, 2095 (1994)
466. S.F. Boys, F. Bernardi, Molec. Phys. **19**, 553 (1970)
467. M. Gutowski, J.G. G.M van der Rijdt, J.H van Lenthe, F.B. van Duijneveldt, J. Chem. Phys. **98**, 4728 (1993)
468. A. Gruneich, B.A. Hess, Theor. Chem. Acc. **100**, 253 (1998)
469. S.D. Kenny, A.P. Horsfield, H. Fujitami, Phys. Rev. B **62**, 4899 (2000)
470. http://www.physik.uni-frankfurt.de/ engel/ncpp.html
471. A.P. Christiansen, Y.S. Lee, K.S. Pitzer, J. Chem. Phys. **71**, 4445 (1970)
472. D.R. Hamann, M. Schlüter, C. Chiang, Phys. Rev. Lett. **43**, 1494 (1979)
473. J.C. Phillips, L. Kleinman, Phys. Rev. **116**, 287 (1959)
474. L. Kleinman, D.M. Bylander, Phys. Rev. Lett. **48**, 1425 (1982)
475. M.I. Petrashen, I.V. Abarenkov, A.A. Berezin, R.A. Evarestov, phys. stat. sol. (b) **40**, 9, 433 (1970)
476. I.V. Abarenkov, V. Heine, Philos. Mag. **12**, 529 (1965)
477. D. Vanderbilt, Phys. Rev. B **41**, 7892 (1990)
478. M. Fuchs, M. Scheffer, Comput. Phys. Commun. **119**, 67 (1999)
479. A. Alkauskas, A. Baratoff, C. Bruder, J. Phys. Chem. A **108**, 6863 (2004)
480. M. Krauss, W.J. Stevens, Ann. Rev. Phys. Chem. **35**, 357 (1984)
481. M. Dolg, in *Modern Methods and Algorithms of Quantum Chemistry*, ed. J. Grotendost, NIC Series, **1**, 479 (2000), **3**, 507 (2000), online http://www.fz-juelich.de/nic-series/NIC-Series-e.html
482. A.V. Titov, N.S. Mosyagin, arXiv.org/physics/0008239 (2000)
483. P.J. Hay, W.R. Wadt, J. Chem. Phys. **52**, 270, 284, 299 (1985)

484. P. Durand, J.C. Barthelat, Theor. Chim. Acta **38**, 283 (1975)
485. W.J. Stevens, H. Basch, M. Krauss, J. Chem. Phys. **81**, 6026 (1984)
486. W.J. Stevens, M. Krauss, H. Basch, P.J. Jasic, Can. J. Phys. **70**, 612 (1992)
487. H. Stoll, B. Metz, M. Dolg, J. Comput. Chem. **23**, 767 (2002)
488. I.V. Abarenkov, I.I. Tupitsyn, J. Chem. Phys. **115**, 1650 (2004)
489. *Electronic Properties of Solids Using Cluster Methods*, eds. T.A. Kaplan, S.D. Mahanti, (Plenum Press, New York London, 1994)
490. I.V. Abarenkov, I.M. Antonova, Int. J. Quantum Chem. **100**, 649 (2004)
491. S. Goedecker, K. Maschke, Phys. Rev. B **42**, 8858 (1990)
492. P.E. Blochl, Phys. Rev. B **41**, 5414 (1999)
493. X. Gonze, R. Stumpf, M. Scheffer, Phys. Rev. B **44**, 8503 (1991)
494. A. Khein, Phys. Rev. B **51**, 16608 (1995)
495. X. Gonze, P.Käckell, M. Scheffer, Phys. Rev. B **41**, 12264 (1990)
496. T. Nakajima, T. Yanai, K. Hirao, J. Comput. Chem. **23**, 847 (2002)
497. *Relativistic Electronic Structure Theory, Part I, Fundamentals*, ed. P. Schwerdtfeger, vol. **11** of Theoretical and Computational Chemistry (Elsevier, Amsterdam, 2002)
498. *Relativistic Electronic Structure Theory, Part II, Applications*, ed.P. Schwerdtfeger, vol. **14** of Theoretical and Computational Chemistry (Elsevier, Amsterdam, 2004)
499. T. Saue, T. Helgaker, J. Comput. Chem. **23**, 814 (2002)
500. A.K. Rajagopal, J. Callaway, Phys. Rev. B **7**, 1912 (1973)
501. C. van Wullen, J. Comput. Chem. **23**, 779 (2002)
502. K.G. Dyall, J. Comput. Chem. **23**, 786 (2002)
503. L. Visscher, J. Comput. Chem. **23**, 759 (2002)
504. L. Visscher, O. Visser, H. Aerts, H. Merenga, W.C. Nieuwport, Comput. Phys. Commun. **81**, 120 (1994)
505. T. Saue, K. Fargi, T. Helgaker, O. Gropen, Molec. Phys. **91**, 937 (1997)
506. I.P. Grant, H.M. Quiney, Int. J. Quantum Chem. **80**, 283 (2000)
507. W. Kutzelnigg, Z. Phys. D **15**, 27 (1990)
508. Y.S. Lee, W.C. Ermler, K.S. Pitzer, J. Chem. Phys. **67**, 5861 (1977)
509. E. Lenthe, E.J. Baerends, J.G. Snijders, J. Chem. Phys. **99**, 4597 (1993)
510. W.C. Ermler, R.B. Ross, P.A. Christiansen, Adv. Quantum Chem. **19**, 139 (1988)
511. P. Schwerdtfeger, in *Theoretical Chemistry and Physics of Heavy and Superheavy elements*, eds. U. Kaldor, S. Wilson (Kluwer, Dordrecht, 2003)
512. A.N. Petrov, N.S. Mosyagin, A.V. Titov, I.I. Tupitsyn, J. Phys. B **37**, 4621 (2004)
513. K.G. Dyall, J. Chem. Phys. **100**, 2118 (1994)
514. A.V. Titov, N.S. Mosyagin, Int. J. Quantum Chem. **71**, 359 (1999)
515. G. Treurich, N.A. Hill, Phys. Rev. B **64**, 073106 (2001)
516. D.Figgen, G. Rauhut, M. Dolg, H. Stoll, Chem. Phys. **311**, 227 (2005)
517. M. Dolg, Theor. Chem. Acc. **114**, 297 (2005)
518. K.A. Peterson, C. Puzzarini, Theor. Chem. Acc. **114**, 283 (2005)
519. X. Cao, M. Dolg, J. Mol. Struct. (Theochem) **673**, 203 (2004)
520. X.Cao, M. Dolg, H. Stoll, J. Chem. Phys. **118**, 487 (2003)
521. V. Bonifacic, S. Huzinaga, J. Chem. Phys. **60**, 2779 (1974)
522. S. Katsuki, S. Huzinagaa, Chem. Phys. Lett. **152**, 203 (1988)
523. L. Seijo, Z. Barandiaran in *Relativistic Electronic Structure Theory, Part II, Applications*, ed.P. Schwerdtfeger, vol. **14** of Theoretical and Computational Chemistry (Elsevier, Amsterdam, 2004), p.417
524. N.S. Mosyagin, A.V. Titov, E. Eliav, U. Kaldor, J. Chem. Phys. **115**, 2007 (2001)
525. N.S. Mosyagin, A.V. Titov, J. Chem. Phys. **122**, 234106 (2005)
526. L.F. Pacios, P.A. Christiansen, J. Chem. Phys. **82**, 2664 (1985)

527. M.G. Kozlov, V.I. Fomichev, Y.Y. Dmitriev, L.N. Labzovsky, A.V. Titov, J. Phys. B **20**, 4939 (1987)
528. Y.Y. Dmitriev, Y.G. Khait, M.G. Kozlov, L.N. Labzovsky, A.O. Mitrushenkov, A.V. Titov, Phys. Lett. A **167**, 280 (1992)
529. A.V. Titov, N.S. Mosyagin, V.F. Ezhov, Phys. Rev. Lett. **77**, 5346 (1996)
530. N.S. Mosyagin, M.G. Kozlov, A.V. Titov, J. Phys. B **31**, L763 (1998)
531. M.G. Kozlov, A.V. Titov, N.S. Mosyagin, P.V. Souschko, Phys. Rev. A **56**, R3326 (1997)
532. A.N. Petrov, N.S. Mosyagin, T.A. Isaev, A.V. Titov, V.F. Ezhov, E. Eliav, U. Kaldor, Phys. Rev. Lett. **88**, 073001 (2002)
533. T.A. Isaev, A.N. Petrov, N.S. Mosyagin, A.V. Titov, E. Eliav, U. Kaldor, Phys. Rev. A **69**, R03050 (2004)
534. A.N. Petrov, A.V. Titov, T.A. Isaev, N.S. Mosyagin, D.P. DeMolle, Phys. Rev. A **72**, 022505 (2005)
535. T.A. Isaev, N.S. Mosyagin, A.N. Petrov, A.V. Titov, Phys. Rev. Lett. **95**, 163004 (2005)
536. P.E. Blöchl, Phys. Rev. B **50**, 17953 (1994)
537. A.V. Titov, N.S. Mosyagin, A.N. Petrov, T.A. Isaev, Int. J. Quantum Chem. **104**, 223 (2005)
538. J. Almlöf, P.R. Taylor, J. Chem. Phys. **86**, 4070 (1987)
539. B. Liu, A.D. McLean, J. Chem. Phys. **91**, 2348 (1989)
540. A.V. Titov, Int. J. Quantum Chem. **45**, 7 (1993)
541. S. Suzuki, K. Nakao, J. Phys. Soc. Jpn. **68**, 1982 (1999)
542. J.C. Boettger, Phys. Rev. B **57**, 8743 (1998)
543. K. Kudin, G.E. Scuseria, R.L. Martin, Phys. Rev. Lett. **89**, 266402 (2002)
544. T. Tsuchiya, M. Abe, T. Nakajama, K. Hirao, J. Chem. Phys. **115**, 4463 (2001)
545. E. van Lenthe, E.J. Baerends, J. Comput. Chem. **24**, 1142 (2003)
546. J.C. Boettger, Eur. Phys. J. **36**, 15 (2003)
547. J.J. Ladik, J. Mol. Struct. (Theochem) **391**, 1 (1997)
548. M. Douglas, N.M. Kroll, Ann. Phys. **82**, 89 (1974)
549. B.A. Hess, Phys. Rev. A **33**, 3742 (1986)
550. J.E. Peralta, G.E. Scuseria, J. Chem. Phys. **120**, 5875 (2004)
551. T. Nakajima, K. Hirao, J. Chem. Phys. **113**, 7786 (2000)
552. A. Wolf, M. Reiher, B.A. Hess, J. Chem. Phys. **117**, 9215 (2002)
553. N.J.M. Geipel, B.A. Hess, Chem. Phys. Lett. **273**, 62 (1997)
554. J.C. Boettger, Phys. Rev. B **57**, 8743 (1998)
555. M.D. Jones, J.C. Boettger, R.C. Albers, D.J. Singh, Phys. Rev. B **61**, 4644 (2000)
556. J.C. Boettger, A.K. Ray, Int. J. Quantum Chem. **90**, 1470 (2002)
557. J.C. Boettger, Int. J. Quantum Chem. **95**, 380 (2003)
558. J.C. Boettger, Int. J. Quantum Chem. **100**, 845 (2004)
559. J.Yang, M. Dolg, Theor. Chem. Acc. **113**, 212 (2005)
560. E.R. Batista, R.L. Martin, P.J. Hay, J. Chem. Phys. **121**, 2144 (2004)
561. J.E. Paralta, J. Uddin, G.E. Scuseria, J. Chem. Phys. **122**, 084108 (2005)
562. P.H.T. Phillipsen, E. van Lenthe, J.G. Snijders, E.J. Baerends, Phys. Rev. B **56**, 13556 (2000)
563. P.H.T. Phillipsen, E.J. Baerends, Phys. Rev. B **61**, 1773 (2000)
564. D.Olguin, M. Cardona, A. Cantarero, Solid State Commun. **122**, 575 (2002)
565. M. Cardona, M.L. Thewalt, Revs. Mod. Phys. **77**, 1173 (2005)
566. L. Colombo, La Rivista del Nuovo Cimento **28**, 1 (2005)
567. C.M. Goringe, D.R. Bowler, E. Hernandez, Rep. Progr. Phys. **60**, 1447 (1997)
568. R. Dovesi, B. Civalleri, R. Orlando, C. Roetti, V.R. Saunders, Rev. Comput. Chem. **21**, 1 (2005)
569. S.G. Semenov, Vestnik LGU, **N16**, 119 (1973)

570. I. Mayer, Int. J. Quantum Chem. **29**, 73 (1986)
571. R.A. Evarestov, V.A. Veryazov, Theor. Chim. Acta **81**, 95 (1991)
572. R.A. Evarestov, V.A. Veryazov, Rev. Solid State Sci. **5**, 415 (1991)
573. R.C. Bochicchio, H.F. Reale, J.A. Medrano, Phys. Rev. B **40**, 7186 (1989)
574. V.A. Veryazov, A.V. Leko, R.A. Evarestov, Phys. Solid State **41**, 1286 (1999)
575. R.A. Evarestov, A.I. Panin, Int. J. Quantum Chem. **88**, 472 (2002)
576. R.C. Bochicchio, H.F. Reale, J. Phys. B **26**, 4871 (1993)
577. R.A. Evarestov, A.I. Panin, Phys. Solid State **42**, 59 (2000)
578. R.C. Bochicchio, Theochem **429**, 229 (1998)
579. R.C. Bochicchio, L.Lain, A. Torre, J. Comput. Chem. **24**, 1902 (2003)
580. R.C. Bochicchio, L.Lain, A. Torre, Chem. Phys. Lett. **374**, 567 (2003)
581. R.A. Evarestov, V.A. Veryazov, phys. stat. sol. (b) **157**, 281, **158**, 201 (1990)
582. J. Choisnet, R.A. Evarestov, I.I. Tupitsyn, V.A. Veryazov, phys. stat. sol. (b) **179**, 441 (1993)
583. R.A. Evarestov, I.I. Tupitsyn, V.A. Veryazov, Int. J. Quantum Chem. **52**, 295 (1994)
584. J. Sichel, M.A. Whitehead, Theor. Chim. Acta **11**, 220 (1968)
585. I.D. Brown, J. Solid State Chem. **82**, 122 (1989)
586. I.D. Brown, J. Chem. Educat. **77**, 1070 (2000)
587. I.D. Brown, J. Appl. Crystallogr. **29**, 479 (1996)
588. I.D. Brown, in *Structure and Bonding in Crystals*, eds. M.O. Keffe, A. Navrotsky, vol. **2**, 1 (Academic Press, New York, 1981)
589. P. Marksteiner, P. Blaha, K. Schwarz, Z. Phys. B: Condens. Matter **64**, 119 (1986)
590. W.Y. Ching, Y.N. Xu, K.W. Wong, Phys. Rev. B **40**, 7684 (1989)
591. P. Saalfrank, M.A. Abdel-Raouf, J. Ladik, R.F. Wood, Phys. Rev. B **41**, 8824 (1990)
592. G.H. Hander, P.J. Brown, J. Spalek, J.M. Monig, Phys. Rev. B **40**, 4463 (1989)
593. J. Choisnet, J.M. Bassat, H. Pilliere, P. Odier, M. Leblanc, Solid State Commun. **66**, 1245 (1988)
594. I.D. Brown, Acta Crystallogr. B **48**, 553 (1992)
595. M. Crespin, C. Landorn, P. Odier, J.M. Bassat, P. Mouron, J. Choisnet, J. Solid State Chem. **100**, 281 (1992)
596. P. Reinhardt, B.A. Hess, M. Causa, Int. J. Quantum Chem. **58**, 297 (1996)
597. J. Muscat, V. Swamy, N.M. Harrison, Phys. Rev. B **65**, 224112 (2002)
598. M.Catti, C. Sandrone, R. Dovesi, Phys. Rev. B **55**, 16122 (1997)
599. M.Catti, G. Sandrone, Faraday Disc. **106**, 189 (1997)
600. R.A. Evarestov, A.I. Panin, phys. stat. sol. (b) **214**, R5 (1999)
601. M.D. Segall, R. Stah, C.J. Pickard, M.C. Payne, Phys. Rev. B **52**, 1005 (1996)
602. R.A. Evarestov, A.V. Leko, V.A. Veryazov, phys. stat. sol. (b) **203**, R3 (1997)
603. R.A. Evarestov, D.E. Usvyat, V.P. Smirnov, Solid State Commun. **127**, 423 (2003)
604. R.A. Evarestov, D.E. Usvyat, V.P. Smirnov, Phys. Solid State **45**, 459 (2003)
605. R.A. Evarestov, V.P. Smirnov, D.E. Usvyat, Theor. Chem. Acc. **114**, 19 (2005)
606. S. Piskinov, E. Heifets, R. Eglitis, G. Borstel, Comput. Mater. Sci. **29**, 165 (2004)
607. M. Veithen, X. Gonze, M. Chosez, Phys. Rev. B **66**, 235113 (2002)
608. R.A. Evarestov, V.P. Smirnov, I.I. Tupitsyn, D.E. Usvyat, Int. J. Quantum Chem. **104**, 110 (2005)
609. W.C. Lu, C.Z. Wang, T.L. Chan, K. Ruedenberg, K.M. Ho, Phys. Rev. B **70**, 041101 (2004).
610. A. Bert, M. Llunell, R. Dovesi, C.M. Zicovich-Wilson, Phys. Chem. Chem. Phys. **5**, 5319 (2003)
611. R.A. Evarestov, I.I. Tupitsyn, A.V. Bandura, V.E. Alexandrov, Int. J. Quantum Chem. **106**, 2191 (2006)
612. V.P. Smirnov, R.A. Evarestov, Phys. Rev. B **72**, 075138 (2005)
613. R.A. Evarestov, A.V. Bandura, V.E. Alexandrov, Phys. Solid State **47**, 2248 (2005)

614. R.A. Evarestov, A.V. Bandura, V.E. Alexandrov, E.A. Kotomin, phys. stat. sol. (b) **242**, R11 (2005)
615. S. Gennard, F. Cora, C.R.A. Catlow, J. Phys. Chem. B **103**, 10158 (1999)
616. E. Mete, R. Shattaf, S. Ellialtioglu, Phys. Rev. B **68**, 035119 (2003)
617. D.Sanchez-Portal, E. Artacho, J.M. Soler, Solid State Commun. **95**, 685 (1995)
618. D.Sanchez-Portal, E. Artacho, J.M. Soler, J. Phys.: Condens. Matter **8**, 3859 (1995)
619. I.I. Tupitsyn, R.A. Evarestov, V.P. Smirnov, Phys. Solid State **47**, 1837 (2005)
620. C.Y. Ren, S.H. Chiou, J. Choisnet, J. Appl. Phys. **99**, 23706 (2006)
621. J.S. Lin, A. Quteish, M.C. Payne, V. Heine, Phys. Rev. B **47**, 4174 (1993)
622. E. Ruiz, S. Alvarez, P. Alemany, Phys. Rev. B **56**, 7189 (1997)
623. R.A. Evarestov, D.E. Usvyat, V.P. Smirnov, Phys. Solid State **45**, 2072 (2003)
624. P.A. Cox, *Transition Metal Oxides* (Carendon Press, Oxford, 1992)
625. C.N.R. Rao, B. Raveau, *Transition Metal Oxides* (VCH Publishers, New York, 1995)
626. W.E. Pickett, Rev. Mod. Phys. **61**, 433 (1989)
627. N.M. Harrison, V.R. Saunders, R. Dovesi, W.C. Mackrodt, A.S. Alexandrov, C.N.R. Rao, J.N. Murrell, R.L. Johnston, D.E. Logan, Philos. Trans. Roy. Soc.London A **356**, 75 (1998)
628. M.D. Towler, N.L. Allan, N.M. Harrison, V.R. Saunders, W.C. Mackrodt, E. Apra, Phys. Rev. B **50**, 5041 (1994)
629. M. Catti, G. Valerio, R. Dovesi, Phys. Rev. B **51**, 7441(1995)
630. M. Catti, G. Sandrone, G. Valerio, R. Dovesi, J. Phys. Chem. Solids **57**, 1735 (1996)
631. A. Chartier, P. DArco, R. Dovesi, V.R. Saunders, Phys. Rev. B **60**, 14042 (1999)
632. E. Ruiz, M. Llunell, P. Alemany, J. Solid State Chem. **176**, 400 (2003)
633. I.d.P.R. Moreira, R. Dovesi, Phys. Rev. B **67**, 134513 (2003)
634. Y.-S. Su, T.A. Kaplan, S.D. Mahanti, J.F. Harrison, Phys. Rev. B **61**, 1324 (2000)
635. M. Nicastro, C.H. Patterson, Phys. Rev. B **65**, 205111 (2002)
636. G. Trimarchi, N. Binggeli, Phys. Rev. B **71**, 035101 (2005)
637. P. Pavindra, A. Kjekshus, H. Fjellvag, A. Delin, O. Eriksson, Phys. Rev. B **65**, 064445 (2002)
638. D.Munoz, N.M. Harrison, F. Illas, Phys. Rev. B **69**, 085115 (2004)
639. R.A. Evarestov, E.A. Kotomin, Yu. A. Mastrikov, D.Gryaznov, E. Heifets, J. Maier, Phys. Rev. B **72**, 124411 (2005)
640. N.N. Kovaleva, A.V. Boris, C. Bernhard, A. Kulakov, A. Pimenov, A.M. Balbashov, G. Khaliullin, B. Keimer, Phys. Rev. Lett. **93**, 147204 (2004)
641. F. Moussa, M. Hennion, J. Rodriguez-Carvajal, H. Moudden, L. Pinsard, A. Revcolevschi, Phys. Rev. B **54**, 15149 (1996)
642. N. Hamada, H. Sawada, I. Solovyev, K. Terakura, Physica **B237238**, 11 (1997)
643. R. Lorenz, R. Hafner, D. Spisak, J. Hafner, J. Magn. Reson., Ser. A **226230**, 889 (2001)
644. P. Ravindran, A. Kjekshus, H. Fjellvag, A. Delin, O. Eriksson, Phys. Rev. B **65**, 064445 (2002)
645. T. Saitoh, A.E. Boquet, T. Mizokawa, H. Namatame, A. Fujimori, M. Abbate, Y. Takeda, M. Takano, Phys. Rev. B **51**, 13942 (1995)
646. TH. Lonkai, D.G. Tomuta, U. Amann, J. Ihringer, R.W.A. Hendrikx, D.M. Tobbens, J.A. Mydosh, Phys. Rev. B **69**, 134108 (2004)
647. M. Fiebig, D.Frolich, K. Kohn, St. Leute, T.H. Lottermoser, V.V. Pavlov, R.V. Pisarev, Phys. Rev. Lett. **84**, 5620 (2000)
648. D.G. Tomuta, S. Ramakrishnan, G.J. Nieuwenhuys, J.A. Mydosh, J. Phys.: Condens. Matter **13**, 4543 (2001)
649. C. Degenhardt, M. Fiebig, D.Frolich, TH. Lottermoser, R.V. Pisarev, Appl. Phys. B **73**, 139 (2001)
650. M.C. Qian, J. Dong, Q. Cheng, Phys. Lett. A **270**, 96 (2000)

651. J.E. Medvedeva, V.I. Anisimov, M.A. Korotin, O.N. Mryasov, A.J. Freeman, J. Phys.: Condens. Matter **12**, 4947 (2000)
652. A.M. Kalashnikova, R.V. Pisarev, JETP Lett. **78**, 3 (2003)
653. T. Bredow, K. Jug, R.A. Evarestov, phys. stat. sol. (b) **243**, R10 (2006)
654. M. Bieringer, J.E. Greedan, J. Solid State Chem. **143**, 132 (1999)
655. J. Park, J.-G. Park, G.S. Jeon, H.Y. Choi, C. Lee, W. To, R. Bewley, K.A. McEwen, T.G. Perring, Phys. Rev. B **68**, 104426 (2003).
656. P. Pulay, Mol. Phys. **17**, 197 (1969)
657. H.B. Schlegel, Theor. Chem. Acc. **103**, 294 (2000)
658. S. Hirata, H. Tori, M. Tatsumi, Phys. Rev. B **57**, 11994 (1998)
659. D.Jacquemin, J.M. Andre, B. Champagne, J. Chem. Phys. **111**, 5306, 5324 (1999)
660. B. Civalleri, Ph.D'Arco, R. Orlando, V.R. Saunders, R. Dovesi, Chem. Phys. Lett. **348**, 131 (2001)
661. K. Doll, V.R. Saunders, N.M. Harrison, Int. J. Quantum Chem. **82**, 1 (2001)
662. K. Doll, Comput. Phys. Commun. **137**, 74 (2001)
663. K. Doll, R. Dovesi, R. Orlando, Theor. Chem. Acc. **112**, 394 (2004)
664. K. Doll, R. Dovesi, R. Orlando, Theor. Chem. Acc., published online, (2005)
665. R. Dovesi, Lecture Notes in Chem. **67**, 179 (1996)
666. K. Rosciszewski, K. Doll, B. Paulus, P. Fulde, Phys. Rev. B **57**, 14667 (1998)
667. *Handbook of Chemistry and Physics*, ed. R.C. Weast, CRC, Boca Raton, FL (1987)
668. B.J. Kennedy, C.J. Howard, B.C. Chakoumakos, Phys. Rev. B **59**, 4023 (1999)
669. F. Pascale, C.M. Zicovich-Wilson, F. Lopez, B. Civalleri, R. Orlando, R. Dovesi, J. Comput. Chem. **25**, 888 (2004)
670. S. Baroni, S. de Gironcoli, A.Dal Corso, P. Giannozzi, Rev. Mod. Phys. **73**, 515 (2001)
671. K. Parlinski, Z.Q. Li, Y. Kawazoe, Phys. Rev. Lett. **78**, 4063 (1997)
672. P. Sikora, J. Phys. Chem. Solids **66**, 1069 (2005)
673. B. Montanari, B. Civalleri, C.M. Zicovich-Wilson, R. Dovesi, Int. J. Quantum Chem. **106**, 1703 (2006)
674. M. Principe, F. Pascale, C.M. Zicovich-Wilson, V.R. Saunders, R. Orlando, R. Dovesi, Phys. Chem. Miner. **31**, 559 (2004)
675. P. Umari, A. Pasquarello, A. Dal Corso, Phys. Rev. B **63**, 094305 (2001)
676. B. Montanari, N.M. Harrison, Chem. Phys. Lett. **364**, 528 (2002)
677. S. Na-Phattalung, M.F. Smith, K. Kim, M.H. Du, S.H. Wei, S.B. Zhang, S. Limpijumnong, Phys. Rev. B **73**, 125205 (2006)
678. R.A. Evarestov, in *Computational Materials Science*, NATO Science Series III, **187**, 122 (2003)
679. R.A. Evarestov, phys. stat. sol. (a) **202**, 235 (2005)
680. R.A. Evarestov, S. Piskunov, E.A. Kotomin, G. Borstel, Phys. Rev. B **67**, 064101 (2003)
681. R.A. Evarestov, V.P. Smirnov, phys. stat. sol. (b) **201**, 75 (1997)
682. R.A. Evarestov, P.W.M. Jacobs, A.V. Leko, Phys. Rev. B **54**, 8969 (1996)
683. R.A. Evarestov, V.P. Smirnov, phys. stat. sol. (b) **215**, 949 (1999)
684. C. Freyria-Fava, R. Dovesi, V.R. Saunders, M.Leslie, C. Roetti, J. Phys.: Condens. Matter **5**, 4793 (1993)
685. L.N. Kantorovich, J.M. Holender, M.J. Gillan, Surf. Sci. **343**, 221 (1995)
686. C.W.M. Castelone, S. Mirb, Phys. Rev. B **70**, 175202 (2004)
687. C. Pisani, Phase Trans. **52**, 123 (1994)
688. M. Leslie, M.J. Gillan, J. Phys. C: Solid State Phys. **18**, 973 (1985)
689. G. Makov, M.C. Payne, Phys. Rev. B **51**, 4014 (1995)
690. J. Lento, J.L. Mozos, R.M. Nieminen, J. Phys.: Condens. Matter **14**, 2637 (2002)
691. U. Gerstmann, P. Deak, R. Rurali, B. Aradi, TH. Frauenheim, H. Overhof, Physica B **340-342**, 190 (2003)
692. C.W.M. Castletone, A. Hoglund, S. Mirbt, Phys. Rev. B **73**, 035215 (2006)

693. J. Shim, E.Lee, Y. Lee, R.M. Niemenen, Phys. Rev. B **71**, 035206 (2005)
694. J.M. Vail, D.Schindel, A. Yang, O. Penner, R. Pandy, S.H. Jiang, M. Blanco, A. Costales, J. Phys. C: Condens. Matter **16**, 3371 (2004)
695. A. Gulans, R.A. Evarestov, I. Tale, phys. stat. sol. (c) **2**, 507 (2005)
696. C. Sousa, Coen de Graaf, F. Illas, Phys. Rev. B **62**, 10013 (2000)
697. R.A. Evarestov, A.R. Sokolov, A.V. Leko, V.A. Veryazov, J. Phys.: Condens. Matter **1**, 6611 (1989)
698. B.T. Plachenov, A.R. Sokolov, R.A. Evarestov, Fiz. Tverdogo Tela **28**, 867 (1986)
699. A.V. Bandura, R.A. Evarestov, phys. stat. sol. (b) **64**, 635 (1974)
700. O. Daniliv, L. Kantorovich, J. Phys. C:Condens. Matter **16**, 7233 (2004)
701. C. Pisani, F. Cora, R. Nada, S. Casassa, Comp. Phys. Commun. **82**, 139 (1994)
702. C. Pisani, U. Birkenheuer, Comp. Phys. Commun. **96**, 221 (1996)
703. C.Pisani, U. Birkenheuer, C. Casassa, F. Cora, EMBED01 User's Manual, University of Torino, Torino (1999)
704. V. Sulimov, S. Casassa, C. Pisani, J. Garapon, B. Poumelle, Modeling Simul. Mater. Sci. Eng. **8**, 763 (2000)
705. E. Scorza, U. Birkenheuer, C. Pisani, J. Chem. Phys. **107**, 9645 (1997)
706. C. Pisani, F. Cora, R. Dovesi, R. Orlando, J. Elect. Spectrosc. Relat. Phenom. **69**, 1 (1994)
707. http://wgc.chem.pu.ru/ valera/cndo/manual.html
708. T. Brudevoll, E.A. Kotomin, N.E. Christensen, Phys. Rev. B **53**, 7731 (1996)
709. Y.N. Hu, Z.Q. Gu, X.F. Zhong, W.Y. Ching, Phys. Rev. B **56**, 7277 (1997)
710. A. Stashans, E. Kotomin, J.L. Calais, Phys. Rev. B **49**, 14854 (1994)
711. I. Tanaka, K. Tatsumi, M. Nakano, H. Adachi, J. Am. Ceram. Soc. **85**, 68 (2002)
712. K. Matsunaga, T. Tanaka, T. Yamamoto, Y. Ikuhara, Phys. Rev. B **68**, 085110 (2003)
713. F. Janetzko, R.A. Evarestov, T. Bredow, K. Jug, phys. stat. sol. (b) **241**, 1032 (2004)
714. F. Janetzko, T. Bredow, K. Jug, J. Chem. Phys. **116**, 8994 (2002)
715. M. Catti, G. Valerio, R. Dovesi, M. Causa, Phys. Rev. B **49**, 14179 (1994)
716. W. Choi, A. Termin, M.R. Hoffmann, J. Phys. Chem. **98**, 13669 (1994)
717. D.Morris, R. Dixon, F.H. Jones, Y. Dou, R. Egdell, S.W. Downes, G. Beamson, Phys. Rev. B **55**, 16083 (1997)
718. T. Umebayashi, T. Yamaki, H. Itoh, K. Asai, J. Phys. Chem. Solids **63**, 1909 (2002)
719. L.A. Errico, G. Fabricius, M. Renteria, Z. Naturforsch. **55**, 267 (2000)
720. A. Stashans, S. Llunell, R. Bergstrom, A. Hagfeldt, S. Lundquist, Phys. Rev. B **53**, 159 (1996)
721. A. Stashans, S. Llunell, R.W. Grimes, J. Phys. Chem. Solids **57**, 1293 (1996)
722. R.I. Eglitis, E.A. Kotomin, G. Borstel, Defects Diffus. Forum **226-228**, 169 (2004), online at http://www.scientific.net
723. H. Donnerberg, A. Birkholz, J. Phys.: Condens. Matter **12**, 8239 (2000)
724. H. Moriwake, Int. J. Quantum Chem. **99**, 824 (2004)
725. A. Shigemi, T. Wada, Jpn. J. Appl. Phys. **43B**, 6793 (2004)
726. J.P. Buban, H. Iddir, S. Ogut, Phys. Rev. B **69**, R180102 (2004)
727. S.A. Prosandeyev, A.V. Fisenko, A.I. Riabchinski, I.A. Osipenko, I.P. Raevski, N. Safontsera, J. Phys.: Condens. Matter **8**, 6705 (1996)
728. J. Robertson, J. Appl. Phys. **93**, 1054 (2003)
729. T. Tanaka, K. Matsunaga, Y. Ikuhara, T. Yamamoto, Phys. Rev. B **68**, 205213 (2003)
730. J. Carrasco, F. Illas, N. Lopez, E.A. Kotomin, Yu. F. Zhukovskii, S. Piskunov, J. Maier, K. Hermansson, phys. stat. sol. (c) **2**, 153 (2005)
731. D.Ricci, G. Bano, G. Pacchioni, F. Illas, Phys. Rev. B **68**, 224105 (2003)
732. R.A. Evarestov, E.A. Kotomin, Yu. F. Zhukovskii, Int. J. Quantum Chem. **106**, 2173 (2006)
733. P.A. Cox, *Transition Metal Oxides*; Clarendon Press, Oxford, UK (1995)

734. R. Astala, P.D. Bristowe, Simul. Mater. Sci. Eng. **9**, 415 (2001)
735. K. Szot, W. Speier, R. Carius, U. Zastrow, W. Beyer, Phys. Rev. Lett. **88**, 075508 (2002)
736. D.E. Usvyat, R.A. Evarestov, V.P. Smirnov, Int. J. Quantum Chem. **100**, 352 (2004)
737. R. Moos, K.H. Saerdtl, J. Am. Ceram. Soc. **80**, 2549 (1997)
738. D.Ricci, G. Bano, G. Pacchioni, F. Illas, Phys. Rev. B **68**, 224105 (2003)
739. J. Crawford, P.W.M. Jacobs, Solid State Chem. **144**, 423 (1999)
740. G. Kresse, J. Hafner, VASP Guide, University of Vienna, Austria, 2003
741. M.G. Brik, J. Phys. Chem. Solids **67**, 856 (2006)
742. F.M. Michel-Calendini, K.A. Muller, Solid State Commun. **40**, 255 (1981)
743. M.O. Selme, P. Pecheur, G. Toussaint, J. Phys. C: Solid State Phys. **17**, 5185 (1984)
744. H. Donnerberg, Phys. Rev. B **50**, 9053 (1994)
745. A.V. Postnikov, A.I. Poteryaev, G. Borstel, Ferroelectrics **206**–**207**, 69 (1998)
746. R.I. Eglitis, A.V. Postnikov, G. Borstel, phys. stat. sol. (b) **209**, 187 (1998)
747. I.I. Tupitsyn, A. Deineka, V.A. Trepakov, L. Jastrabik, S.E. Kapphan, Phys. Rev. B **64**, 195111 (2001)
748. R.K. Astala, P.D. Bristowe, Model. Simul. Mater. Sci. Eng. **12**, 79 (2004)
749. R. Waser, T. Bieger, J. Maier, Solid State Commun. **76**, 1077 (1990)
750. J. Fleig, K.D. Kreuer, J. Maier, in *Handbook of Advanced Ceramics*, Elsevier, Singapore, 2003, p.57
751. G. Banach, W.M. Temmerman, Phys. Rev. B **69**, 054427 (2004)
752. H. Zenia, G.A. Gehring, G. Banach, W.M. Temmerman, Phys. Rev. B **71**, 024416 (2005)
753. J. Geck, P. Wochner, D.Bruns, B. Buchner, U. Gebhardt, S. Kiele, P. Reutler, A. Revcolevschi, Phys. Rev. B **69**, 104413 (2004)
754. D.Fuks, L. Bakaleinikov, E.A. Kotomin, J. Felsteiner, A. Gordon, R.A. Evarestov, D. Gryaznov, J. Maier, Solid State Ion. **177**, 217 (2006)
755. J.K. Perry, J. Tahir-Kheli, W.A. Goddard III, Phys. Rev. B **63**, 144510 (2001)
756. D.Fuks, S. Dorfman, S. Piskunov, E.A. Kotomin, Phys. Rev. B **71**, 014111 (2005)
757. D.Fuks, S. Dorfman, E.A. Kotomin, Yu. Zhukovskii, A.M. Stoneham,Phys. Rev. Lett. **85**, 4333 (2000)
758. D.Fuks, S. Dorfman, J. Felsteiner, L. Bakaleinikov, A. Gordon, E.A. Kotomin, Solid State Ion. **173**, 107 (2004)
759. L. Rormark, S. Stolen, K. Wik, T. Grande, J. Solid State Chem. **163**, 186 (2002)
760. A.G. Kchachaturyan, *Theory of Structural Transformations in Solids*, Wiley, New York, 1983
761. *International Tables for Crystallography, volume E, Subperiodic Groups*, eds. V. Kopsky, D.B. Litvin (Kluwer Academic Publishers, Dodrecht/Boston/London, 2002)
762. V. Kopsky, Acta Cryst. A **45**, 805, 816 (1989)
763. V. Kopsky, Acta Cryst. A **56**, 370 (2000)
764. E.A. Wood, Bell Telephone Tech. J. **43**, 541 (1964)
765. V.P. Smirnov, P. Tronc, Phys. Solid State **48**, 1295 (2006)
766. C. Noguera, *Physics and Chemistry at Oxide Surfaces*, Cambridge Univeristy Press (1996)
767. C. Noguera, J. Phys.: Condens. Matter **12**, R367 (2000)
768. F. Finocchi, F. Bottin, C. Noguera, in *Computational Materials Science*, eds. C.R.A. Catlow, E.A. Kotomin, IOS Press, 2003, p.196
769. T. Bredow, G. Geudtner, K. Jug, J. Chem. Phys. **105**, 6395 (1996)
770. R.A. Evarestov, T. Bredow, K. Jug, Phys. Solid State **43**, 1774 (2001)
771. T. Bredow, K. Jug, Chem. Phys. Lett. **223**, 89 (1994)
772. P.W. Tasker, J. Phys. C: Solid State Phys. **12**, p (1979)
773. J.C. Boettger, Phys. Rev. B **49**, 16798 (1994)

774. V. Fiorentini, M.J. Methfesse, J. Phys.: Condens. Matter **8**, 6525 (1996)
775. L. Fu, E. Yaschenko, L. Resta, Phys. Rev. B **60**, 2697 (1999)
776. R.A. Evarestov, A.V. Bandura, Int. J. Quantum Chem. **100**, 452 (2004)
777. R.A. Evarestov, A.V. Bandura, Int. J. Quantum Chem. **96**, 282 (2002)
778. L.N. Kantorovich, M.J. Gilan, Surf. Sci. **374**, 373 (1997)
779. P. Reinhardt, B. Hess, Phys. Rev. B **50**, 12015 (1994)
780. R.A. Evarestov, V.P. Smirnov, D.E. Usvyat, Int. J. Quantum Chem. **104**, 102 (2005)
781. G. Fernandes-Cata, L.G. Alvarez, R. Dovesi, C.M. Zicovich-Wilson, J. Phys. Chem. B **106**, 7316 (2004)
782. S.P. Bates, G. Kresse, M.G. Gillan, Surf. Sci. **385**, 386 (1997)
783. U. Diebold, Surf. Sci. Rep. **48**, 53 (2003)
784. M. Calatayud, B. Mguig, C. Minot, Surf. Sci. **526**, 297 (2003)
785. M. Calatayud, A. Markovits, M. Menetrey, B. Mguig, C. Minot, Catal. Today **85**, 125 (2003)
786. M. Menetrey, A. Markovits, C. Minot, G. Pacchioni, J. Phys. Chem. B **108**, 12858 (2004)
787. C. Noguera, F. Finocci, J. Goniakowski, J. Phys.: Condens. Matter **16**, S2509 (2004)
788. T. Bredow, L. Giordano, F. Cinquini, G. Pacchioni, Phys. Rev. B **70**, 035419 (2004)
789. M. Calatayud, C. Minot, Surf. Sci. **552**, 169 (2004)
790. A.V. Bandura, D.G. Sykes, V. Shapovalov, T.N. Truong, J.D. Kubicki, R.A.Evarestov, J. Phys. Chem. B **108**, 7844 (2004)
791. A.V. Bandura, J.O. Sofo, J.D. Kubicki, J. Phys. Chem. B **110**, 8386 (2006)
792. S.J. Thompson, S.P. Lewis, Phys. Rev. B **73**, 073403 (2006)
793. K.J. Hameeuw, G. Cantele, D.Ninno, F. Trani, G. Iadonisi, J. Chem. Phys. **124**, 024708 (2006)
794. M.L. Sushko, A.Yu. Gal, A.L. Shluger, J. Phys. Chem. B **110**, 4853 (2006)
795. G.U. von Oertzen, A.R. Gerson, Int. J. Quantum Chem. **106**, 2054 (2006)
796. P. Persson, A. Stashans, R. Bergstrom, S. Lunell, Int. J. Quantum Chem. **70**, 1055 (1998)
797. K. Jug, G. Geudtner, J. Mol. Cat. A **119**, 143 (1997)
798. T. Brinkley, M. Dietrich, T. Engel, P. Farral, G. Gantner, A. Schafer, A. Szuchmacher, Surf. Sci. **395**, 292 (1998)
799. N.M. Harrison, X.G. Wang, J. Muskat, M. Scheffer, Faraday Discuss. **114**, 305 (1999)
800. J. Leconte, A. Markovits, M.K. Skalli, C. Minot, A. Belmajdoub, Surf. Sci. **497**, 194 (2002)
801. E.V. Stefanovich, T.N. Truong, J. Phys. Chem. B **102**, 3018 (1998)
802. J. Goniakowski, M.J. Lindan, Surf. Sci. **350**, 145 (1996)
803. P.J.D. Lindan, N.M. Harrison, J.M. Holender, M.J. Gillan, Phys. Rev. Lett. **80**, 762 (1998)
804. G. Charlton, P.B. Howes, C.L. Nickin, P. Steadman, J.S.G. Taylor, C.A. Muryn, S.P. Harte, J. Mercer, R. McGrath, D. Norman, T.S. Turner, G. Thornton, Phys. Rev. Lett. **78**, 495 (1997)
805. E.V. Stefanovich, T.N. Truong, Chem. Phys. Lett. **299**, 623 (1999)
806. T.T. Rantala, T.S. Rantala, V. Lannto, Surf. Sci. **420**, 103 (1999)
807. J. Oviedo, M.J. Gillan, Surf. Sci. **463**, 93 (2000)
808. I. Manassidis, J. Goniakowski, L.N. Kantorovich, M.J. Gillan, Surf. Sci. **339**, 258 (1995)
809. J. Goniakowski, M.J. Gillan, Surf. Sci. **350**, 145 (1996)
810. S.P. Bates, Surf. Sci. **512**, 29 (2002).
811. P.J.D. Lindan, Chem. Phys. Lett. **328**, 325 (2000)
812. M. Calatayud, J. Andrus, A. Beltrn, Surf. Sci. **430**, 213 (1999)
813. F. Ciriaco, L. Cassidei, M. Cacciatore, G. Petrella, Chem. Phys. **303**, 55 (2004)
814. M. Melle-Franco, G. Pacchioni, Surf. Sci. **461**, 54 (2000)

815. F.R. Sensato, R. Custdio, M. Calatayud, A. Beltron, J. Andrus, J.R. Sambrano, E. Longo, Surf. Sci. **511**, 408 (2002)
816. R.A. Evarestov, A.V. Bandura, E.V. Proskurov, phys. stat. sol. (b) **243**, 1823 (2006)
817. A.V. Postnikov, P. Entel, P. Ordejon, Phase Trans. **75**, 143 (2002)
818. Y. Yamaguchi, K. Tabata, T. Yashima, J. Mol. Struct. (Theochem) **714**, 221 (2005)
819. H. Szuber, G. Czempik, R. Larciprete, B. Adamowicz, Sens. Actuators B Chem. **70**, 177 (2000)
820. J.M. Themlin, R. Sporken, J. Darville, R. Caudano, J.M. Gilles, R.L. Johnson, Phys. Rev. B **42**, 11914 (1990).
821. A.L. Dawar, J.C. Joshi, J. Mater. Sci. **19**, 1 (1984)
822. V.A. Gercher, D.F. Cox, Surf. Sci. **322**, 177 (1995)
823. T. Hiemstra, H. Yong, W.H. van Riemsdijk, Langmuir **15**, 5942 (1999)
824. S. Piskunov, E.A. Kotomin, E. Heifets, J. Maier, R.I. Eglitis, G. Borstel, Surf. Sci. **575**, 75 (2005)
825. R.A. Evarestov, A.V. Bandura, V.E. Alexandrov, phys. stat. sol. (b) **246**, 1013 (2006)
826. N. Erdman, K.R. Poeppelmeier, M. Asta, O. Warschkow, D.E. Ellis, L.D. Marks, Nature **419**, 55 (2002)
827. A. Ikeda, T. Nishimura, T. Morishita, Y. Kido, Surf. Sci. **433–435**, 520 (1999).
828. G. Charlton, S. Brennan, C.A. Muryn, R. McGrath, D.Norman, T.S. Turner, G. Thornton, Surf. Sci. **457**, L376 (2000).
829. J. Padilla, D. Vanderbilt, Surf. Sci. **418**, 64 (1998)
830. N.V. Krainyukova, V.V. Butskii, Surf. Sci. **454**, 628 (2000)
831. E. Heifets, R.I. Eglitis, E.A. Kotomin, J. Maier, G. Borstel, Phys. Rev. B **64**, 235417 (2001)
832. E. Heifets, R.I. Eglitis, E.A. Kotomin, J. Maier, G. Borstel, Surf. Sci. **513**, 211 (2002)
833. A. Asthagiri, D.S. Sholl, Phys. Rev. B **73**, 125432 (2006)
834. K. van Benthem, C. Elsässer, J. Appl. Phys. **90**, 6156 (2001)
835. Y.S. Lee, J.S. Lee, T.W.Noh, D.Y. Byun, K.S. Yoo, K. Yamaura, E.T. Muromachi, Phys. Rev. B **67**, 113101 (2003).
836. Z.Q. Li, J.L. Zhu, C.Q. Wu, Z. Tang, Y. Kawazoe, Phys. Rev. B **58**, 8075 (1998)
837. S. Kimura, J. Yamauchi, M. Tsukada, S. Watanabe, Phys. Rev. B **51**, 11049 (1995)
838. Yu. F. Zhukovskii, S. Piskunov, E.A. Kotomin, O. Sychev, G. Borstel, Microelectr. Eng. **81**, 467 (2005)
839. S. Piskunov, E.A. Kotomin, E.Heifets, Microelectr. Eng. **81**, 472 (2005)
840. S. de Lazaro, E. Longo, J.R. Sambrano, A. Bertran, Surf. Sci. **552**, 149 (2004)
841. X.Y. Hue, C.L. Wang, W.L. Zhong, Surf. Sci. **550**, 73 (2004)
842. G. Borstel, R.I. Eglitis, E.A. Kotomin, E. Heifets, phys. stat. sol.(b) **236**, 253 (2003)
843. N. Erdman, L.D. Marks, Surf. Sci. **526**, 107 (2003)
844. R. Bader, *Atoms in Molecules: A Quantum Theory*, Oxford University Press, New York, 1990
845. A. Asthagiri, D.S. Sholl, J. Chem. Phys. **116**, 9914 (2002)
846. A. Stashans, F. Erazo, J. Ortiz, P. Valverde, Philos. Mag. B **81**, 1977 (2001)
847. Z. Fang, K. Terakura, Surf. Sci. **470**, L75 (2000)
848. J. Carrasco, F. Illas, N.Lopez, E.A. Kotomin, Yu. F. Zhukovskii, R.A. Evarestov, Yu. A. Mastrikov, S. Piskunov, J. Maier, Phys. Rev. B **73**, 064106 (2006)
849. J. Carrasco, J.R.B. Gomes, F. Illas, Phys. Rev. B **69**, 064116 (2004)
850. P. Mori-Sanchez, J.M. Recio, B. Silvi, C. Sousa, A.M. Pendas, V. Luana, F. Illas, Phys. Rev. B **66**, 075103 (2002)
851. R.A. Evarestov, E.A. Kotomin, E. Heifets, J. Maier, G. Borstel, Solid State Commun. **127**, 367 (2003)
852. R.A. Evarestov, E.A. Kotomin, D.Fuks, J. Felsteiner, J. Maier, Appl. Surf. Sci. **238**, 457 (2004)

853. E. Heifets, E.A. Kotomin, J. Maier, Phys. Chem. Chem. Phys. **5**, 4180 (2003)
854. F. Bottin, F. Finocchi, C. Noguera, Phys. Rev. B **68**, 035418 (2003)
855. R.A. Evarestov, E.A. Kotomin, Yu. A. Mastrikov, D.Gryaznov, E. Heifets, J. Maier, Phys. Rev. B **72**, 214411 (2005)
856. http://www.supercomputing.it/software.php?cat=11
857. http://www.msg.ku.edu/ msg/MGM/links/comp.html
858. http://www.redbrick.dcu.ie/ noel/linux4chemistry
859. J.V. Vondele, M. Crack, F. Mohamed, M. Parrinello, T. Chassaing, J. Hutter, Comp. Phys. Commun. **167**, 103 (2005)
860. C. Pisani, J. Mol. Struct.(Theochem), **463**, 125 (1999)
861. R. Orlando, R. Dovesi, P. Ugliengo, C. Roetti, V.R. Saunders, Int. J. Inorg. Mater. **1**, 147 (1999)
862. R. Dovesi, R. Orlando, C. Roetti, C. Pisani, V.R. Saunders, phys. stat. sol. (b) **217**, 63 (2000)
863. C. Pisani, R. Dovesi, C. Roetti, M. Causa, R. Orlando, S. Casassa, V.R. Saunders, Int. J. Quantum Chem. **77**, 1032 (2000)
864. G.Te Velde, F.M. Bickelhaupt, E.J. Baerends, C.F. Guerra, S.J.A. VAN Gisbergen, J.G. Snijders, T. Ziegler, J. Comput. Chem. **22**, 931 (2001)
865. A.E. Mattson, P.A. Schultz, M.P. Desjarlais, T.R. Mattsson, K. Leung, Model. Simul. Mater. Sci.Eng. **13**, R1 (2005)
866. B. Delley, J. Chem. Phys. **113**, 7756 (2000)
867. H. Eschrig, K. Koepernik, I.Chaplygin, J. Solid State Chem. **176**, 482 (2003)
868. S.D. Kenny, A.P. Horsfield, H. Fujitani, Phys. Rev. B **62**, 4899 (2000)
869. R.A. Evarestov, I.I. Tupitsyn, V.A. Veryazov, Int. J. Quantum Chem. **52**, 295 (2004)
870. J.J.P. Stewart, J. Mol. Mod. **10**, 155 (2004)
871. L. Kantorovich, A. Stashans, E. Kotomin, P.W.M. Jacobs, Int. J. Quantum Chem. **52**, 1177 (1994)
872. B. Civalleri, F. Napoli, Y. Noel, C. Roetti, R. Dovesi, Cryst. Eng. Commun. **8**, 364 (2006), see online www.rsc.org/crystengcomm
873. http://www.ccr.jussieu.fr/ccr/Documentation/Calcul/ XCRYSDEN/Documentation.html
874. A. Kokalj, Comput. Mater. Sci. **28**, 155 (2003)
875. http://www.ivec.org/GULP/

Index