

István Mayer
scientific publications

1. I. MAYER: Simple Calculation of Proton Hyperfine Splitting in C–H Bond. (In Hungarian.) *Magy. Kém. Foly.* **76**, 607–614 (1970)
2. I. N. KOMAR', O. T. NIKOLOV and I. MAYER: On the Structure and Stability of Free Radicals Formed in the γ -Irradiated Glycine. (In Russian.) *Teor. Eksp. Khim.* **6**, 561–566 (1970)
3. I. MAYER: On the Derivation of the Hartree–Fock Equations. *Acta Phys. Hung.* **30**, 373–379 (1971)
4. I. MAYER: Comments on the EPR Spectra of Irradiated Solid Glycine. *Chem. Phys. Letters* **8**, 117–119 (1971)
5. I. MAYER: Derivation of the Extended Hartree–Fock Equations. *Chem. Phys. Letters* **11**, 397–400 (1971)
6. I. MAYER: On the Conditions of Applicability of Bodenstein's Principle. (In Hungarian.) *Magy. Kém. Foly.* **77**, 302–304 (1971)
7. I. MAYER and M. SIMONYI: On the Concept of the Complex with Relatively Long Lifetime in Bimolecular Reactions. *Acta Chim. Hung.* **71**, 149–158 (1972)
8. L. SÜMEGI, I. MAYER, I. KENDE and F. TÜDÖS: Chemistry of Free Radicals IX. EPR Study of Some Ortho-Substituted Phenyl-Nitrogen-Oxide Radicals. (In Hungarian.) *Magy. Kém. Foly.* **78**, 254–256 (1972)
9. I. MAYER: On the Derivation of the Hartree–Fock Equations II. *Acta Phys. Hung.* **34**, 83–96 (1973)
10. I. MAYER, J. LADIK and G. BICZÓ: Spin Projected Extended Hartree–Fock Equations. *Internat. J. Quantum Chem.* **7**, 583–608 (1973)
11. I. MAYER: On the Generalized Brillouin Theorem for Spin Projected Wave Functions. *Acta Phys. Hung.* **34**, 305–309 (1973)
12. I. MAYER: Some Remarks on “Statistical Theories of Chemical Reactions. Distribution in the Transition Region” *J. Chem. Phys.* **60**, 2564–2565 (1974)

13. I. MAYER: On the Derivation of the Hartree–Fock Equations III. Introduction of the LCAO Formalism. *Acta Phys. Hung.* **36**, 11–17 (1974)
14. I. MAYER: Spin Projected Extended Hartree–Fock Equations II. Odd–Electron Systems. *Internat. J. Quantum Chem.* **8**, 893–899 (1974)
15. I. MAYER: On the Derivation of the Extended Hartree–Fock Equations, I. A Simple Derivation Using Specified Variations. *Acta Phys. Hung.* **37**, 39–52 (1974)
16. I. MAYER: Spin Projected EHF Method: Calculations for a Four–Electron Model System. *Internat. J. Quantum Chem.* **8**, 363–372 (1974)
17. I. N. KOMAR’, O. T. NIKOLOV and I. MAYER: Structure of the Free Radicals Formed in the γ -Irradiated γ -Glycine. (In Russian.) *Teor. Eksp. Khim.* **10**, 839–844 (1974)
18. I. MAYER, J. KONDÁSZ: Spin–Projected EHF method II. The Equations for Successive Optimization of the Orbitals in the Many-Electron Case. *Internat. J. Quantum Chem.* **9**, 517–526 (1975)
19. I. MAYER, M. KERTÉSZ: Spin–Projected EHF Method III. Applications to π -Electron Systems. *Internat. J. Quantum Chem.* **9**, 527–536 (1975)
20. I. MAYER: Comparative Studies on Model Potential Curves. *Acta Phys. Hung.* **39**, 133–141 (1975)
21. M. SIMONYI, I. MAYER: Barrier Width: a Powerful Parameter for Hydrogen Transfer Reactions. *J.C.S. Chem. Comm.* **1975**, 695–696 (1975)
22. M. SIMONYI, I. MAYER: A Critical Survey on the Transition State Theory. *Acta Chim. Hung.* **87**, 15–32 (1975)
23. I. MAYER: Application of Quantum Chemistry for Investigating Elementary Reactions. (In Hungarian.) *Kém. Közl.* **44**, 480–486 (1975)
24. I. MAYER, M. KERTÉSZ: A Comparison of Different DODS Methods when the Number of Electrons Increases. *Internat. J. Quantum Chem.* **10**, 961–966 (1976)
25. I. MAYER: The Extended Hartree–Fock Method. (In Hungarian.) *Kém. Közl.* **46**, 397–402 (1976)
26. R. BARS, I. MAYER: Model-Reference Control of Systems Identified by the Laguerre Orthonormal Structure. “*Identification and System Parameter Estimation*” (ed. N.S. Rajbman) v. III., 430–443 (Moscow, 1976)

27. R. BARS, I. MAYER: Algorithms for Evaluating the Laguerre and x Expansion Coefficients of Transfer Functions. *Probl. Control and Information Theory* **6**, 249–260 (1977)
28. I. MAYER, S. A. ANGELOV: Refined LCAO Treatment of Superexchange in Insulators. *Physica* **95B**, 93–98 (1978)
29. I. MAYER: Spin-Projected EHF Method IV. Comparison of Potential Curves Given by Different One-Electron Methods. *Internat. J. Quantum Chem.* **14**, 29–38 (1978)
30. I. MAYER, I. HARGITTAI: On the Structural Differences Between Trifluoromethyl Sulphonyl Chloride ($\text{CF}_3\text{SO}_2\text{Cl}$) and Methane Sulphonyl Chloride ($\text{CH}_3\text{SO}_2\text{Cl}$). *Z.Naturforsch.* **34A**, 911–913 (1979)
31. I. MAYER, S. A. ANGELOV: EHF Description of Superexchange: Relations to Anderson's Model. *Internat. J. Quantum Chem.* **18**, 783–796 (1980)
32. I. MAYER: The Spin Projected Extended Hartree–Fock Method. *Advances Quantum Chem.* **12**, 189–262 (1980)
33. B. P. VAN EIJCK, I. HARGITTAI, I. MAYER: The Molecular Conformation of Benzene Sulphonyl Chloride. *J.Mol.Struct.* **69**, 301–303 (1980)
34. I. MAYER, M. RÉVÉSZ: Nonorthogonal Localized Orbitals.(In Hungarian). *Kém. Közl.* **54**, 205–212 (1980)
35. I. MAYER, S. ANGELOV: The Mechanism of Participation of Non-magnetic B-site Cations in the Superexchange in spinels. *Phys. stat. solidi (b)* **106**, 467–471 (1981)
36. P. R. SURJÁN, M. RÉVÉSZ, I. MAYER: Strictly Localized Molecular Orbitals. *J.C.S. Faraday Trans. II.* **77**, 1129–1131 (1981)
37. P. R. SURJÁN, I. MAYER: Delocalization Corrections to the Strictly Localized Molecular Orbitals: A Linearized SCF Approximation. *Theor. Chim. Acta* **59**, 603–607 (1981)
38. M. SIMONYI, I. MAYER: Formal Similarity Between Irreversible and Reversible Bimolecular Kinetics. *React. Kinet. Catal. Lett.* **18**, 431–432 (1981)
39. I. MAYER: Non-orthogonal Localized Orbitals to Study Delocalization Effects. *Chem. Phys. Letters* **89**, 390–394 (1982)
40. P. R. SURJÁN, I. MAYER, M. KERTÉSZ: Localization and Delocalization: Distinction between Through Space and Through Bond Interactions. *J. Chem. Phys.* **77**, 2454–2459 (1982)

41. P. R. SURJÁN, G. NÁRAY-SZABÓ, I. MAYER: Conformational Analysis by Bond Orbitals with Delocalization Corrections: Rotation of the Ser-195 Side Chain in α -Chymotrypsin. *Internat. J. Quantum Chem.* **22**, 929–938 (1982)
42. I. MAYER, M. RÉVÉSZ: Warning to the Users of the “GEOMO” Program System. *Comput. and Chem.* **6**, 153–154 (1982)
43. I.MAYER: Towards a “Chemical” Hamiltonian. *Internat. J. Quantum Chem.* **23**, 341–363 (1983)
44. I.MAYER: Charge, Bond Order and Valence in the Ab Initio SCF Theory. *Chem. Phys. Letters* **97**, 270–274 (1983)
45. I.MAYER, M. RÉVÉSZ, I. HARGITTAI: On the C-S Bond Length Variations and *d*-Orbital Participation in Some Sulphonyl Chloride Derivatives. *Acta Chim. Hung.* **114**, 159–172 (1983)
46. I. MAYER: On the Behaviour of the UHF Method Near the “Critical” Point. *Acta Phys. Hung.* **54**, 249–266 (1983)
47. I. MAYER, S. A. ANGELOV: On the Interference of Superexchange Interactions. *J. Phys.C. Solid State Phys.* **16**, L857–L858 (1983)
48. I. MAYER, M. RÉVÉSZ: Bond Orders and Valences in Some Simple Sulphur Compounds. *Inorg. Chim. Acta* **77**, L205–L206 (1983)
49. I. MAYER, S. A. ANGELOV: On the Ground State of Antiferromagnets at Zero Temperature. *Solid State Comm.* **49**, 593–595 (1984)
50. I. MAYER, P. R. SURJÁN: Localization and Delocalization II: Role of Overlap in Interbond Interactions. *J. Chem. Phys.* **80**, 5649–5658 (1984)
51. I. MAYER: Bond Order and Valence: Relations to Mulliken’s Population Analysis. *Internat. J. Quantum Chem.* **26**, 151–154 (1984)
52. I. MAYER: Comments on the Quantum Theory of Valence and Bonding: Choosing between Alternative Definitions. *Chem. Phys. Letters* **110**, 440–444 (1984)
53. I. MAYER, P. R. SURJÁN: Hypervalency and the Sulphur *d*-Orbital Problem. *Acta Chim. Hung.* **117**, 85–87 (1984)
54. M. SIMONYI, I. MAYER: A Deductive Approach to Elementary Chemical Kinetics. *Educ. Chem.* **22**, 52–53 (1985)
55. S. ANGELOV, I. MAYER: The Ground State of the Heisenberg Hamiltonian in Four-Spin Systems with Antiferromagnetic Coupling. *Acta Phys. Hung.* **58**, 161–167 (1985)

56. I. MAYER, S. ANGELOV: Simple Estimation of Ground-state Energy of Antiferromagnets. *Solid State Comm.* **54**, 437–439 (1985)
57. I. MAYER: Bond Orders and Valences in the SCF Theory: A Comment. *Theor. Chim. Acta* **67**, 315–322 (1985)
58. P. R. SURJÁN, I. MAYER, I. LUKOVITS: Second–Quantization–Based Perturbation Theory for Intermolecular Interactions without Basis Set Superposition Error. *Chem. Phys. Letters* **119**, 538–542 (1985)
59. P. R. SURJÁN, I. MAYER, I. LUKOVITS: The Interaction of Chemical Bonds II. Ab Initio Theory for Overlap, Delocalization and Dispersion Interactions. *Phys. Rev.* **A32**, 748–755 (1985)
60. M. A. ATANASOV, S. ANGELOV, I. MAYER: Angular Dependence of Superexchange Interactions in σ -Bonded Transition Metal Clusters. *Solid State Comm.* **56**, 743–745 (1985)
61. I. MAYER: Simple Constructive Proof of Karadakov’s Extended Pairing Theorem. *Internat. J. Quantum Chem.* **29**, 31–34 (1986)
62. I. MAYER: On Bond Orders and Valences in the Ab Initio Quantum Chemical Theory. *Internat. J. Quantum Chem.* **29**, 73–84 (1986)
63. I. MAYER: Bond Order and Valence Indices in the Ab Initio Quantum Chemistry. (In Hungarian.) *Kém. Közl.* **65**, 383–412 (1986)
64. I. MAYER: Bond Orders and Valences from Ab Initio Wave Functions. *Internat. J. Quantum Chem.* **29**, 477–483 (1986)
65. I. MAYER: “*Chapters of Quantum Chemistry*” (textbook for postgraduate teaching; in Hungarian) pp. 172, Mérnöktovábbképző Int., Budapest, 1987.
66. I. MAYER: Bond Orders and Valences: Role of d -Orbitals for Hypervalent Sulphur. *J. Mol. Struct. (Theochem)* **149**, 81–89 (1987)
67. I. MAYER: On the Chemical Hamiltonian Approach, Bond Orders and Valences. pp 145–159 in “*Modelling of structure and properties of molecules*” (ed. Z.B.Maksić), Ellis Horwood, Chichester, 1987.
68. I. MAYER, Á. VIBÓK: SCF Theory of Intermolecular Interactions without Basis Set Superposition Error. *Chem. Phys. Letters* **136**, 115–121 (1987)
69. I. MAYER: On the Non-additivity of the Basis Set Superposition Error and how to Prevent its Appearance. *Theor. Chim. Acta* **72**, 207–210 (1987)
70. I. MAYER, Á. VIBÓK: Intermolecular SCF Method without BSSE: the Closed–Shell Case. *Chem. Phys. Letters* **140**, 558–564 (1987)

71. I. MAYER: The “Chemical Hamiltonian Approach” and the SCF Method. *J. Mol. Struct. (Theochem)* **165**, 255–272 (1988)
72. I. MAYER, Á. VIBÓK: SCF Equations in the Chemical Hamiltonian Approach. *Chem. Phys. Letters* **148**, 68–72 (1988)
73. I. MAYER: Some Remarks on the Polemic about “Direct Consequences of the Bond Index Statistical Interpretation” *Chem. Phys. Letters* **148**, 95–96 (1988)
74. P. R. SURJÁN, I. MAYER, R. POIRIER: Second Quantization and the Hellmann–Feynman Theorem: a Unified View on Energy Derivatives. *J. Mol. Struct. (Theochem)* **170**, 1–7 (1988)
75. Á. VIBÓK, I. MAYER: Intermolecular SCF Theory without BSSE: the Equations and Some Applications for Small Systems. *J. Mol. Struct. (Theochem)* **170**, 9–17 (1988)
76. M. RÉVÉSZ, I. BERTÓTI, G. MINK, I. MAYER: ON the Use of “Pseudo-Atoms” in Cluster Calculations for Modelling Molecular Fragments, Solids and Surfaces. *J. Mol. Struct. (Theochem)* **181**, 335–343 (1988)
77. I. MAYER: Bond Orders in Three–Centre Bonds: an Analytical Investigation into the Electronic Structure of Diborane and the Three–Centre Four–Electron Bonds of Hypervalent Sulphur. *J. Mol. Struct. (Theochem)* **186**, 43–52 (1989)
78. M. ATANASOV, S. ANGELOV, I. MAYER: Modelling of Angular Dependence of Superexchange: Application to Copper(II) Dimers. *J. Mol. Struct. (Theochem)* **187**, 23–33 (1989)
79. I. MAYER, P. R. SURJÁN: Improved Intermolecular SCF Theory and the BSSE Problem. *Internat. J. Quantum Chem.* **36**, 225–240 (1989)
80. I. MAYER, P. R. SURJÁN, Á. VIBÓK: BSSE-Free SCF Methods for Intermolecular Interactions. *Internat. J. Quantum Chem. Quantum Chem. Symp.* **23**, 281–290 (1989)
81. Á. VIBÓK, I. MAYER: Towards a Third Order Perturbation Theory of Intermolecular Interactions Without BSSE. *Acta Phys. Hung.* **68**, 241–251 (1990)
82. P. R. SURJÁN, I. MAYER: Intermolecular Interactions: Biorthogonal Perturbation Theory Revisited. *J. Mol. Struct. (Theochem)* **226**, 47–58 (1991)
83. I. MAYER, L. TÚRI: An Analytical Investigation into the BSSE Problem. *J. Mol. Struct. (Theochem)* **227**, 43–65 (1991)

84. I. MAYER, Á. VIBÓK: A BSSE-Free SCF Algorithm for Intermolecular Interactions. *Internat. J. Quantum Chem.* **40**, 139–148 (1991)
85. I. MAYER: Some Remarks on the Maximum Bond Order. *Theor. Chim. Acta* **79**, 377–378 (1991)
86. P. R. SURJÁN, I. MAYER: Second Quantization and Exchange Perturbation Theory for Intermolecular Interactions. The Basis Set Superposition Error Problem. *J. Mol. Struct. (Theochem)* **232**, 51–63 (1991)
87. I. MAYER, Á. VIBÓK: A Comparison of a Priori and a Posteriori BSSE Correction Schemes for Rare Gas–Proton Potential Curves. *Acta Phys. Hung.* **70**, 403–413 (1991)
88. I. MAYER, I. LUKOVITS, T. RADNAI: Hydration of Cations: H-Bond Shortening as an Electrostatic Effect. *Chem. Phys. Letters* **188**, 595–598 (1992)
89. I. MAYER: The LCAO Representation of the First Order Density Matrix in Non-Orthogonal Basis Sets: a Note. *J. Mol. Struct. (Theochem)* **255**, 1–7 (1992)
90. I. MAYER, P. R. SURJÁN: Monomer Geometry Relaxation and the Basis Set Superposition Error. *Chem. Phys. Letters* **191**, 497–499 (1992)
91. M. RÉVÉSZ, I. MAYER: Effect of Oxygen Impurities on the Electronic Structure and Ionization Potential of Polyethylene. *Acta Chim. Hung. – Models in Chemistry* **129**, 287–295 (1992)
92. Á. VIBÓK, I. MAYER: A BSSE-Free SCF Algorithm for Intermolecular Interactions. II. Sample Calculations on Hydrogen-Bonded Complexes. *Internat. J. Quantum Chem.* **43**, 801–811 (1992)
93. I. MAYER: Comment on: Exact Perturbation Treatment of the Basis set Superposition Correction. *J. Chem. Phys.* **97**, 5257–5258 (1992)
94. I. MAYER: On the Additivity and Interference of Interactions. *Internat. J. Quantum Chem. Quantum Chem. Symp.* **26**, 773–779 (1992)
95. P.-O. LÖWDIN, I. MAYER: Some Studies of the General Hartree–Fock method. *Advances Quantum Chem.* **24**, 79–114 (1992)
96. I. MAYER, P.-O. LÖWDIN: Some Comments on the General Hartree–Fock Method. *Chem. Phys. Letters* **202**, 1–6 (1993)
97. P. VALIRON, Á. VIBÓK, I. MAYER: A Comparison of *a posteriori* and *a priori* BSSE Correction Schemes for SCF Intermolecular Energies. *J. Comp. Chem.* **14**, 401–409 (1993)

98. I. MAYER and P. R. SURJÁN: Handling Overlap as a Perturbation. *Croat. Chem. Acta* **66**, 161–165 (1993)
99. I. MAYER and Á. GÖMÖRY: Use of Energy Partitioning for Predicting Primary Mass Spectrometric Fragmentation Steps: A Preliminary Account. *Internat. J. Quantum Chem. Quantum Chem. Symp.* **27**, 599–605 (1993)
100. B. PAIZS and I. MAYER: Coupled Perturbed Hartree-Fock Equations: an Alternative Derivation and Generalization to Non-orthogonal Orbitals. *Chem. Phys. Letters* **220**, 97–101 (1994)
101. J. G. ÁNGYÁN, M. LOOS and I. MAYER: Covalent Bond Orders and Atomic Valence Indices in the Topological Theory of Atoms in Molecules. *J. Phys. Chem.* **98**, 5244–5248 (1994)
102. I. MAYER, Á. VIBÓK and P. VALIRON: A Full CI Investigation into the BSSE Problem. *Chem. Phys. Letters* **224**, 166–174 (1994)
103. I. MAYER and Á. GÖMÖRY: Semiempirical Quantum Chemical Method for Predicting Mass-Spectrometric Fragmentations. *J. Mol. Struct. (Theochem)* **311**, 331–341 (1994)
104. Á. SOMOGYI, V. H. WYSOCKI and I. MAYER: The Effect of Protonation Site on Bond Strengths in Simple Peptides: Application of Ab Initio and MNDO Bond orders and MNDO Energy Partitioning. *J. Am. Soc. Mass Spectrom.* **5**, 704–717 (1994)
105. M. KIENINGER, S. SUHAI and I. MAYER: The Chemical Hamiltonian Approach in Density Functional Theory. *Chem. Phys. Letters* **230**, 485–490 (1994)
106. M. B. RUIZ and I. MAYER: Deriving Gradient Formulae for SCF Methods by Using Brillouin-type Theorems. Gradients in the HPHF Method. *Chem. Phys. Letters* **236**, 217–228 (1995)
107. I. MAYER: Non-orthogonal Localized Orbitals and Orthogonal Atomic Hybrids Derived from Mulliken’s Population Analysis. *Chem. Phys. Letters* **242**, 499–506 (1995)
108. I. MAYER, Á. VIBÓK, G. HALÁSZ and P. VALIRON: A BSSE-Free SCF Algorithm for Intermolecular Interactions. III. Generalization for Three-Body Systems and for Using Bond functions. *Internat. J. Quantum Chem.* **57**, 1049–1055 (1996)
109. I. MAYER: Atomic Orbitals from Molecular Wave Functions: the Effective Minimal Basis. *J. Phys. Chem.* **100**, 6249–6257 (1996)

110. G. HALÁSZ, Á. VIBÓK, P. VALIRON and I. MAYER: A BSSE-Free SCF Algorithm for Treating Several Weakly Interacting Systems. *J. Phys. Chem.* **100**, 6332–6335 (1996)
111. I. MAYER: Orthogonal Effective Atomic Orbitals in the Topological Theory of Atoms. *Canadian J. Chem.* **74**, 939–942 (1996)
112. I. MAYER: On the Hylleraas Functional for a Non-Hermitian Unperturbed Hamiltonian. *Mol. Phys.* **89**, 515–519 (1996)
113. R. PONEC and I. MAYER: Investigation of some Properties of Multicenter Bond Indices. *J. Phys. Chem. A* **101**, 1738–1741 (1997)
114. I. MAYER, G. RÄTHER and S. SUHAI: The Chemical Hamiltonian Approach for Infinite chains. *Chem. Phys. Letters* **270**, 211–216 (1997)
115. I. MAYER: Simple Proof of the Pairing Theorem. *Internat. J. Quantum Chem.* **63**, 31–33 (1997)
116. I. MAYER: The Driving Force Behind the Rules of the Valence Shell Electron Pair Repulsion Model. *Structural Chemistry* **8**, 309–311 (1997)
117. P. VALIRON and I. MAYER: Hierarchy of Counterpoise Corrections for N-body Clusters: Generalization of the Boys-Bernardi Scheme. *Chem. Phys. Letters* **275**, 46–55 (1997)
118. I. MAYER and Á. VIBÓK: BSSE-Free Second Order Intermolecular Perturbation Theory. *Mol. Phys.* **92**, 503–510 (1997)
119. Á. VIBÓK, G. HALÁSZ and I. MAYER: BSSE-Free Second Order Intermolecular Perturbation Theory II. Sample Calculations on Hydrogen-Bonded Complexes. *Mol. Phys.* **93**, 873–877 (1998)
120. I. MAYER: The Chemical Hamiltonian Approach for Treating the BSSE Problem of Intermolecular Interactions. *Internat. J. Quantum Chem.* **70**, 41–63 (1998)
121. I. MAYER and P. VALIRON: Second Order Møller-Plesset Perturbation Theory without Basis Set Superposition Error. *J. Chem. Phys.* **109**, 3360–3373 (1998)
122. I. MAYER, G. RÄTHER and S. SUHAI: Wannier-type Orbitals Derived from Mulliken’s Population Analysis. *Chem. Phys. Letters* **293**, 81–89 (1998)
123. G. LENDVAY and I. MAYER: Some Difficulties in Computing BSSE-Corrected Potential Surfaces of Chemical Reactions. *Chem. Phys. Letters* **297**, 365–373 (1998)

124. G. HALÁSZ, Á. VIBÓK and I. MAYER: Comparison of BSSE-Corrected Perturbation Theories for Calculating Intermolecular Interaction Energies. *J. Comp. Chem.* **20**, 274–283 (1999)
125. A. HAMZA, Á. VIBÓK, G. HALÁSZ and I. MAYER: BSSE-Free SCF Theories: A Comment. *J. Mol. Struct. (Theochem)* **501-502**, 427–434 (2000)
126. I. MAYER: Unitary Perturbation Theory: a Generalization of the Two-by-Two Rotations. *Theor. Chem. Accounts* **104**, 163–166 (2000)
127. I. MAYER: A Chemical Energy Component Analysis. *Chem. Phys. Letters* **332**, 381–388 (2000)
128. S. SAUGE, P. VALIRON and I. MAYER: Dissociative Recombination of Antiprotonic Atomcules $\bar{p}\text{He}^+$ with Positronium: Towards Antyhdrogen Synthesis? *Chem. Phys. Letters* **334**, 330-336 (2001)
129. A. HAMZA and I. MAYER: Overlap Repulsion with Löwdin’s Pairing Theorem. *Internat. J. Quantum Chem.* **82**, 53–59 (2001)
130. A. HAMZA and I. MAYER: Overlap Repulsion with Löwdin’s Pairing Theorem. II. The Leading Term. *Internat. J. Quantum Chem.* **82**, 105–112 (2001)
131. I. MAYER and A. HAMZA: Energy Decomposition in the Topological Theory of Atoms-in-Molecules and in the LCAO formalism: a Note. *Theor. Chem. Accounts* **105**, 360–364 (2001)
132. Z. BIKÁDI, G. KERESZTURY, S. HOLLY, O. EGYED, I. MAYER AND M. SIMONYI: Role of Secondary Interactions in the Conformational Equilibrium of 2,6-Diisopropylphenol. *J. Phys. Chem. A*, **105**, 3471-3474 (2001)
133. P. SALVADOR, M. DURAN and I. MAYER: One- and Two-Center Energy Components in the AIM Theory. *J. Chem. Phys.* **115**, 1153–1157 (2001)
134. I. MAYER and Á. GÖMÖRY: Predicting Primary Mass Spectrometric Cleavages: a ‘Quasi-Koopmans’ ab Initio Approach. *Chem. Phys. Letters* **344**, 553–564 (2001)
135. A. HAMZA, Á. VIBÓK, G.J. HALÁSZ and I. MAYER: Second Order Energy Components in the BSSE-Free Intermolecular Perturbation Theory. *Theor. Chem. Accounts* **107**, 38–47 (2001)
136. G.J. HALÁSZ, Á. VIBÓK, S. SUHAI and I. MAYER: Toward a BSSE-Free Description of Strongly Interacting Systems. *Internat. J. Quantum Chem.* **89**, 190-197 (2002)
137. I. MAYER: On Löwdin’s Method of Symmetric Orthogonalization. *Internat. J. Quantum Chem.* **90**, 63-65 (2002)

138. I. MAYER: Hermitian Fockian in the Chemical Hamiltonian Approach: Filling Löwdin's Prediction. *Internat. J. Quantum Chem.* **90**, 89-91 (2002)
139. A. HAMZA and I. MAYER: Novel Energy Decomposition Schemes for Intermolecular Interactions. *Recent Res. Devel. Quantum Chem.* **3**, 25-49 (2002)
140. Á. VIBÓK, G.J. HALÁSZ and I. MAYER: BSSE-Corrected Perturbation Theories of Intermolecular Interactions. pp. 263–283 in “*Electron Correlations and Materials Properties 2*” (ed. A. Gonis, N. Kioussis and M. Ciftan) Kluwer Academic/Plenum Publishers, New York etc., 2002.
141. I. MAYER and A. HAMZA: Interatomic Exchange Energy Components. *Internat. J. Quantum Chem.* **92**, 174–180 (2003)
142. a) I. MAYER, *Simple Theorems, Proofs, and Derivations in Quantum Chemistry*, pp 352, Kluwer Academic/Plenum Publishers, New York etc., 2003.
 b) I. MAYER, *Izbrannye glavy kvantovoj khimii: Dokazatel'stva teorem i vyvod formul*, pp 384, Binom Laboratoriya Znaniy, Moscow, 2006.
143. A. HAMZA and I. MAYER: Physical Analysis of the Diatomic “Chemical” Energy Components. *Theor. Chem. Accounts* **109**, 91–98 (2003)
144. I. MAYER: An Exact Chemical Decomposition Scheme for the Molecular Energy. *Chem. Phys. Letters* **382**, 265–269 (2003)
145. I. MAYER and P. SALVADOR, Overlap Populations, Bond Orders and Valences for “Fuzzy” Atoms. *Chem. Phys. Letters* **383**, 368–375 (2004)
146. P. SALVADOR and I. MAYER, Energy Partitioning for “Fuzzy” Atoms. *J. Chem. Phys.* **120**, 5046–5052 (2004)
147. P. SALVADOR and I. MAYER, Second order Møller-Plesset perturbation theory without basis set superposition error. II. Open-shell systems. *J. Chem. Phys.* **120**, 5882–5889 (2004)
148. I. MAYER, M. KNAPP-MOHAMMADY and S. SUHAI, Bond Orders and Energy Components in Polymers. *Chem. Phys. Letters* **389**, 34–38 (2004)
149. I. MAYER, Löwdin Population Analysis is not Rotationally Invariant. *Chem. Phys. Letters* **393**, 209–212 (2004)
150. I. MAYER: Interrelations Between the *a priori* and *a posteriori* BSSE-correction Schemes. *Internat. J. Quantum Chem.* **100**, 559–566 (2004)
151. I. PÁPAI, G. SCHUBERT, I. MAYER, G. BESENYEI and M. ARESTA, Mechanistic Details of Nickel(0)-Assisted Oxidative Coupling of CO₂ with C₂H₄. *Organometallics* **23**, 5252–5259 (2004)

152. I. MAYER and A. HAMZA, Treating Nonadditivity as a Perturbation: a Quasi-Particle Formalism. pp. 187–198 in *Fundamental Word of Quantum Chemistry: A tribute volume to the memory of Per-Olov Löwdin* (ed. E.J. Brändas and E.S. Kryachko) vol. III, Kluwer Academic, 2004.
153. I. MAYER and A. HAMZA, Atomic Decompositions of Identity: a General Formalism for Population Analysis and Energy Decomposition. *Internat. J. Quantum Chem.* **103**, 798–807 (2005)
154. G. BRUHN, E.R. DAVIDSON, I. MAYER and A.E. CLARK, Löwdin Population Analysis With and Without Rotational Invariance. *Internat. J. Quantum Chem.* **106**, 2065–2072 (2006)
155. P. SALVADOR, D. ASTURIOL and I. MAYER, A General Efficient Implementation of the BSSE-Free SCF and MP2 Methods Based on the Chemical Hamiltonian Approach. *J. Comp. Chem.* **27**, 1505–1516 (2006)
156. I. MAYER: Energy Partitioning Schemes. *Phys. Chem. Chem. Phys.*, **8**, 4630–4646 (2006)
157. I. MAYER: Bond Order and Valence Indices: A Personal Account. *J. Comp. Chem.* **28**, 204–221 (2007)
158. I. MAYER: Energy Partitioning Schemes: a Dilemma. *Faraday Discussions*, **135**, 439–450 (2007)
159. I. MAYER: Comment on “Analysis on Solvated Molecules with a New Energy Partitioning Scheme for Intra- and Intermolecular Interactions” *J. Phys. Chem. B*, **111**, 669–671 (2007)
160. I. MAYER: Using Singular Value Decomposition for a Compact Presentation and Improved Interpretation of the CIS Wave Functions. *Chem. Phys. Letters* **437**, 284–286 (2007)
161. I. MAYER: Local Spins: an Alternative Treatment for Single Determinant Wave Functions. *Chem. Phys. Letters* **440**, 357–359 (2007)
162. P. SALVADOR and I. MAYER: One- and Two-Center Physical Space Partitioning of the Energy in the Density Functional Theory. *J. Chem. Phys.* **126**, 234113, 1–10 (2007)
163. I. MAYER: Identifying a Pair of Interacting Chromophores by Using SVD Transformed CIS Wave Functions. *Chem. Phys. Letters* **443**, 420–425 (2007)
164. A. L. TCHOUGRÉEFF, A. M. TOKMACHEV and I. MAYER: Towards a Possible *Ab Initio* Molecular Mechanics: Transferability of Density Matrix Elements. *Internat. J. Quantum Chem.* **107**, 2539–2555 (2007)

165. G. TASI and I. MAYER: An Extension of the Virial Theorem for General Wave Functions. *Chem. Phys. Letters* **449**, 221–226 (2007)
166. I. MAYER: Some Formal Aspects of the Theory of Intermolecular Interactions and of the BSSE Problem. *Collect. Czech. Chem. Commun.* **73**, 1391–1414 (2008)
167. I. MAYER: Some Simple Models for the Barrier of Rotation in the Ethane Molecule. (In Hungarian.) *Magy. Kém. Foly.* **114**, 163–165 (2008)
168. I. MAYER, P. SALVADOR: Effective Atomic Orbitals for Fuzzy Atoms. *J. Chem. Phys.* **130**, 234106, 1–6 (2009)
169. D. ASTURIOL, P. SALVADOR and I. MAYER: Dissecting the Hindered Rotation of Ethane. *ChemPhysChem*, **10**, 1987–1992 (2009)
170. I. MAYER: Local Spins: An Improved Treatment for Correlated Wave Functions. *Chem. Phys. Letters*, **478**, 323–326 (2009)
171. I. MAYER: Analytical Derivation of the Hückel “ $4n + 2$ rule”. *Theor. Chem. Accounts*, **125**, 203–206 (2010)
172. I. MAYER and E. MATITO: Calculation of Local Spins for Correlated Wave Functions. *Phys. Chem. Chem. Phys.*, **12**, 11308–11314 (2010)
173. I. MAYER: On the Promotion Energy of an Atom in a Molecule. *Chem. Phys. Letters*, **498**, 366–369 (2010)
174. I. MAYER: Löwdin’s Pairing Theorem and some its Applications. *Mol. Phys.*, **108**, 3273–3278 (2010)
175. T. ZOBOKI and I. MAYER: Extremely Localized Non-Orthogonal Orbitals by the Pairing Theorem. *J. Comp. Chem.*, **32**, 689–695 (2011)
176. I. MAYER, I. BAKÓ and A. STIRLING: Are there Atomic Orbitals in a Molecule? *J. Phys. Chem. A*, **115**, 12733–12737 (2011)
177. I. MAYER: Improved Chemical Energy Component Analysis. *Phys. Chem. Chem. Phys.*, **14**, 337–344 (2012)
178. E. RAMOS-CORDOBA, E. MATITO, I. MAYER and P. SALVADOR: Toward a Unique Definition of the Local Spin. *J. Chem. Theory Comput.*, **8**, 1270–1279 (2012)
179. I. MAYER and T. A. ROKOB: Internal Coordinates of Quantum Mechanical Systems. *Phys. Rev. A*, **85**, 044101 (2012)

180. I. MAYER: Local Spins: Improving the Treatment for Single Determinant Wave Functions. *Chem. Phys. Letters*, **539–540**, 172–174 (2012)
181. I. MAYER: Improved Definition of Bond Orders for Correlated Wave Functions. *Chem. Phys. Letters*, **544**, 83–86 (2012)
182. I. MAYER: Molecular Energy Decompositions. *EPJ Web of Conferences*, **34**, 02002, 1-5 (2012)
183. E. RAMOS-CORDOBA, E. MATITO, P. SALVADOR and I. MAYER: Local Spins: Improved Hilbert-Space Analysis. *Phys. Chem. Chem. Phys.*, **14**, 15291–15298 (2012)
184. I. BAKÓ, A. STIRLING, A. P. SEITSONEN and I. MAYER: Extracting Chemical Information from Plane Wave Calculations by a 3D “Fuzzy Atoms” Analysis. *Chem. Phys. Letters*, **563**, 97–101 (2013)
185. E. RAMOS-CORDOBA, P. SALVADOR and I. MAYER: The Atomic Orbitals of the Topological Atom. *J. Chem. Phys.*, **138**, 214107, 1–9 (2013)
186. I. MAYER: Relation Between the Hilbert Space and “Fuzzy Atoms” Analyses. *Chem. Phys. Letters*, **585**, 198–200 (2013)
187. I. MAYER: Covalent Bonding: The Role of Exchange Effects. *J. Phys. Chem. A*, **118**, 2543–2546 (2014)
188. I. MAYER: Effective Atomic Orbitals: A Tool for Understanding Electronic Structure of Molecules. *Internat. J. Quantum Chem.*, **114**, 1041–1047 (2014)
189. I. MAYER: Hermitian “Chemical” Hamiltonian: an Alternative *ab Initio* Method. *Theor. Chem. Accounts*, **134**, 86, 1–10 (2015)
190. I. MAYER: Restoring Rotational Invariance of Löwdin Populations. *Structural Chemistry*, **27**, 51–55 (2016)
191. I. BAKÓ and I. MAYER: The Hierarchy of the Collective Effects in Water Clusters. *J. Phys. Chem. A*, **120**, 631–638 (2016)
192. I. BAKÓ and I. MAYER: On Dipole Moments and Hydrogen Bond Identification in Water Clusters. *J. Phys. Chem. A*, **120**, 4408–4417 (2016)
193. I. MAYER: *Bond Orders and Energy Components: Extracting Chemical Information from Molecular Wave Functions*. pp.229, CRC Press, Boca Raton–London–New York, 2016/17.
194. I. MAYER and I. BAKÓ: Many-Body Energy Decomposition with Basis Set Superposition Error Corrections. *J. Chem. Theor. Comp.*, **13**, 1883–1886 (2017)