Warsaw, October 7, 2013

CURRICULUM VITAE OF
GRZEGORZ CHAŁASIŃSKI

Total number of papers: 152
Number of citations:
total: 6082
without autocitations: 5012
H-index: 42
10 papers over 100 citations.

I. PERSONAL

A. Date and Place of Birth:
January 1, 1949, Łódź, Poland

B. Business Address:
Faculty of Chemistry
University of Warsaw
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II. EDUCATION

A. M.Sc. (Chemistry) University of Warsaw, Poland, 1972
B. Ph.D. (Chemistry) University of Warsaw, Poland, 1977
C. Habilitation Degree, D. Sc. University of Warsaw, Poland, 1986

III. POSITION HELD

1999 - Full Professor, Faculty of Chemistry, University of Warsaw, Poland

1993-1999 - Associate Professor, Faculty of Chemistry, University of Warsaw, Poland

1977-1993 - Assistant Professor, Faculty of Chemistry, University of Warsaw, Poland

1988 - 1994, 3-month visits each year, visiting professor, Dept. of Chemistry and Biochemistry
Southern Illinois University, Carbondale, USA

1992,1993 - Research Associate (3 months), Dept. of Chemistry, Oakland University, Rochester, USA

1985-1987 - Post-Doctoral Fellow, Dept. of Chemistry, University of Utah, Salt Lake City, USA

1983 - Visiting Professor (3 months), Dept. of Chemistry, University of Utrecht, The Netherlands

1982 - Research Associate (2 months), Dept. of Chemistry, University of Lund, Sweden

1981 - Visiting Professor (3 months), Dept. of Chemistry, University of Utrecht, The Netherlands

1979-1980 - Visiting Professor (1 year), Dept. of Chemistry, University of Utrecht, The Netherlands

1971-1977 - Senior Assistant, Dept. of Chemistry, University of Warsaw, Poland

IV. OTHER APPOINTMENTS:
since 1998 - Affiliate Staff Scientist of Pacific Northwest National Laboratories at Richland, (honorary appointment) Washington, USA,

since 2001 - Adjunct Professor of Oakland University, Michigan, USA (honorary appointment).

V. OTHER POSITIONS:

Dean, Faculty of Chemistry, University of Warsaw, 2002-2008

Research Coordinator of Centre for Preclinical Research and Technology (CePT), Warsaw, Poland, since 2007-

Member of the Senate of University of Warsaw, since 2008 -

Chairman of the Human Resources Senate Committee, 2008-2012

Chairman of the Science and Research Advisory Senate Committee, since 2012 -

Chairman of the Science Advisory Board of Interdisciplinary Center for Mathematical and Computational Modelling, since 2005-

VI. RESEARCH INTERESTS

Theory and computation of intermolecular forces. Applications of quantum mechanical methods, both in the wave function framework and density functional theory, to the study of intermolecular interactions: van der Waals complexes, H-bonded systems, non-additive interactions. DFT methods for non-covalently bound complexes and aggregates. Charge-Transfer excitations in donor-acceptor pairs. Theory of aurophilic interactions.

VII. AWARDS

1988 Joint Prize of the Ministry of Science, Higher Education and Technology (Poland) for research in the field of intermolecular interactions (National Award)
1996 W. Swietoslawski Award, Department of Chemistry, Warsaw University
2001 Jan Zawidzki Medal, Award of Polish Chemical Society
2013 Beneficiary of the MISTRZ Academic Grant for Professors

VIII. MEMBERSHIPS

1. Polish Chemical Society
2. International Society for Theoretical Chemical Physics (National Representative for Poland).
3. American Chemical Society

IX. LIST OF PUBLICATIONS

1. G. Chalasinski, W. Kolos, B. Petelenz, L. Piela, "Gaussian Orbitals in Calculations of the Second-Order Corrections to the Interaction Energy of two Hydrogen Atoms", Chem. Phys. Lett. 12, 233-235 (1971).
2. G. Chalasinski, B. Jeziorski, "Exact Calculation of Exchange Polarization Energy for H2+ Ion", Int. J. Quant. Chem., 7, 63-73 (1973).
3. G. Chalasinski, B. Jeziorski, "Multipole Structure of Exchange Polarization Energy for H2+ Ion", Int. J. Quant. Chem. 7, 745-757 (1973).
4. G. Chalasinski, B. Jeziorski, "An Exact Treatment of the Induction Interaction between the Atoms in the Hydrogen Molecule", Mol. Phys. 27, 649-655 (1974).
5. G. Chalasinski, B. Jeziorski, "On the Exchange Polarization Effects in the Interaction of Two Helium Atoms", Mol. Phys. 32, 81-91 (1976).

6. G. Chalasinski, B. Jeziorski, K. Szalewicz, "On the Convergence Properties of the Rayleigh-Schroedinger and Hirschfelder-Silbey Perturbation Expansion for Molecular Interaction Energies", Int. J. Quant. Chem, 11, 247-257 (1977).
7. G. Chalasinski, B. Jeziorski, J. Andzelm, K. Szalewicz, "On the Multipole structure of Exchange Dispersion Energy in the Interaction of two helium Atoms", Mol. Phys., 33, 971-977 (1977).
8. G. Chalasinski, B. Jeziorski, "Exchange Polarization Effects in the Interaction of Closed-Shell Systems. The Beryllium-Beryllium Interaction", Theoret. Chim. Acta, 46, 277-290 (1977).
9. M. Bulski, G. Chalasinski, "On Basis Set Effects on SCF Calculations of the Interaction Energy between Closed-Shell Atoms", Theoret. Chim. Acta 44, 399-404 (1977).
10. B. Jeziorski, K. Szalewicz, G. Chalasinski,"Symmetry Forcing and Convergence Properties of Perturbation Expansions for Molecular Interaction Energies", Int. J. Quant. Chem. 14, 271-287 (1978).
11. M. Bulski, G. Chalasinski, B. Jeziorski, "Many-Orbital cluster Expansion for the Exchange-Repulsion Energy in the Interaction of Closed-Shell Systems. The Neon-Neon Interaction", Theoret. Chim. Acta, 52, 93-101 (1979).
12. M. Bulski, G. Chalasinski, "Many-Orbital Cluster Expansion for the Exchange-Repulsion Nonadditivity in the Interaction of Rare Gas Atoms. The Neon Trimer", Theor. Chim. Acta, 56, 199-210 (1980).
13. G. Chalasinski, K. Szalewicz, "Degenerate Symmetry-Adapted Perturbation Theory. Convergence Properties of Perturbation Expansion for Excited States of H2+ Ion", Int. J. Quant. chem. 18, 1071-1089 (1980).
14. G. Chalasinski, "Exchange Dispersion Effect in the Interaction between HF Molecules", Chem. Phys. Lett. 86, 165-169 (1982).
15. G. Chalasinski, S. van Smaalen, F. B. van Duijneveldt, "Ab initio Calculations of Exchange Repulsion Between two Ar Atoms", Mol. Phys. 45, 1271-1278 (1982).
16. G. Chalasinski, S. van Smaalen, F. B. van Duijneveldt, "Analysis of Intra-Atomic Correlation Effects on the First-Order Interaction Energy between He Atoms", Mol. Phys. 45, 1113-1124 (1982).
17. M. Bulski, G. Chalasinski, "On Exchange-Repulsion Nonadditivity in the Interaction of Three Argon Atoms", Chem. Phys. Lett. 89, 450-454 (1982).
18. G. Chalasinski, "Perturbation Calculations of the Interaction Energy between Closed-Shell Hartree-Fock Atoms. The Neon Dimer", Mol. Phys., 49, 1353-1373 (1983).
19. G. Chalasinski, "Exchange-Perturbation Calculation of the Interaction Energy between Be Atoms Including Intra-Atomic Correlation Effects", Chem. Phys., 82, 207-213 (1983).
20. M. Gutowski, G. Chalasinski, J. van Duijneveldt-van de Rijdt, "Effective Basis Set for Calculations of Exchange-Repulsion Energy", Int. J. Quant. Chem., 26, 971-982 (1984).
21. G. Chalasinski, J. van Lenthe, T. P. Groen, "An Analysis of the Partial Wave Expansion of the Dispersion Energy for Ne2", Chem. Phys. Lett., 110, 369-374 (1984).
22. G. Chalasinski, M. Gutowski, "Dimer Centered Basis Set in the Calculations of the First-Order Interaction Energy with CI Wave Functions. The He Dimer", Mol. Phys., 54, 1173-1184 (1985).
23. G. Chalasinski, "Intramolecular Correlation Correction to the First-Order Interaction Energy between H2 Molecules and Its Influence on the H2-H2 Potential Surface", Mol. Phys., 57, 427-439 (1986).
24. M. Gutowski, J. van Lenthe, J. Verbeek, F. B. van Duijneveldt, G. Chalasinski, "The Basis Set Superposition Error in Correlated Electronic Structure Calculations", Chem. Phys. Lett., 124, 370-375 (1986).
25. M. Bulski, G. Chalasinski, "Perturbation Claculations of the Nonadditivity of the Exchange-Dispersion Energy for the Be3 System", Chem. Phys. Lett., 128, 25-30 (1986).
26. M. Gutowski, F. B. van Duijneveldt, G. Chalasinski, L. Piela, "Does the Boys and Bernardi Function Counterpoise Actually Overcorrect the Basis Set Superposition Error?", Chem. Phys. Lett., 129, 325-328 (1986).
27. M. Gutowski, J. Verbeek, J. van Lenthe, G. Chalasinski, "The Impact of Higher Polarization Functions on Second-Order Dispersion Energy. Partial Wave Expansion and Damping Phenomenon for He2", Chem. Phys., 111, 271-283 (1987).
28. M. Bulski, G. Chalasinski, "On the Nonadditivity of the Second-Order Exchange-Dispersion Energy in the Interaction of Three Helium Atoms", J. Chem. Phys., 86, 937-946 (1987).
29. M. Gutowski, F. B. van Duijneveldt, G. Chalasinski, L. Piela, "Proper Correction for Basis Set Superposition Error in SCF Calculations of Intermolecular Interactions", Mol. Phys., 61, 233-248 (1987).
30. G. Chalasinski, R. A. Kendall, J. Simons, "Ab Initio Studies of the Structures and Energies of the H-(H2O) and H-(H2O)2 Complexes", J. Chem. Phys., 87, 2965-2975 (1987).

31. G. Chalasinski, D. J. Funk, J. Simons, W. H. Breckenridge, "Moller-Plesset Perturbation Theory for van der Waals Complexes Bound by Electron Correlation Effects: Ground State of the Ar and Mg Dimers", J. Chem. Phys., 87, 3569-3579 (1987).
32. G. Chalasinski, R. A. Kendall, J. Simons, "Ab Initio Studies of the Structure and Energetics of the H-(H2) Complex", J. Phys. Chem, 91, 6151-6158 (1987).
33. G. Chalasinski, M. M. Szczesniak, "On the Connection between Supermolecular Moller-Plesset Treatment of the Interaction Energy and the Perturbation Theory of Intermolecular Forces", Mol. Phys., 63, 205-224 (1988).
34. G. Chalasinski, M. Gutowski, "Weak Interactions between Small Systems. Models for Studying the Nature of Intermolecular Forces and Challenging Problems for Ab Initio Calculations", Chem. Rev., 88, 943-962 (1988).
35. G. Chalasinski, J. Simons, "Van der Waals Minima in Excited States by Means of Moller-Plesset Perturbation Theory: the 3aS+u State of He2 and the 3P State of MgHe", Chem. Phys. Lett., 148, 289-296 (1988).
36. G. Chalasinski, R. A. Kendall, H. Taylor, J. Simons, "Propensity Rules for Vibration-Rotation-Induced Electron Detachment of Diatomic Anions: Application to NH---NH+e-", J. Phys. Chem., 92, 3086-3091 (1988).
37. R. Kendall, J. Simons, M. Gutowski, G. Chalasinski, "The Ab Initio Energy and Structure of H-(H2)2", J. Phys. Chem. 93, 621-625 (1989).
38. D. J. Funk, W. H. Breckenridge, J. Simons, G. Chalasinski, "Moller-Plesset Perturbation Theory Calculation of Alkaline Earth-Rare Gas Complexes: Ground States of Mg-He and Mg-Ar", J. Chem. Phys., 91, 1114-1120 (1989).
39. M. M. Szczesniak, G. Chalasinski, "Anisotropy of Correlation Effects in Hydrogen-Bonded Systems. HF Dimer", Chem. Phys. Lett., 161 532-38 (1989).
40. G. Chalasinski, S. M. Cybulski, M. M. Szczesniak, S. Scheiner, "Analysis of the Potential Energy Surface of Ar-NH3", J. Chem. Phys., 91 7809-17 (1989).
41. G. Chalasinski, S. M. Cybulski, M. M. Szczesniak, S. Scheiner, "Nonadditive Effects in HF and HCl Trimers", J. Chem. Phys., 91 7048-56 (1989).
42. G. Chalasinski, B. Kukawska-Tarnawska, "Ab initio Studies of the Structure and Energies of the NO-He and NO-Ar Complex", J. Phys. Chem., 94 3450-54 (1990).
43. S. M. Cybulski, G. Chalasinski, R. Moszynski, "On Decomposition of MP2 Supermolecular Interaction Energy and Basis Set Effects", J. Chem. Phys., 92 4357 (1990).
44. G. Chalasinski, M. M. Szczesniak, S. M. Cybulski "Calculations of Nonadditive Effects by means of Supermolecular MPPT Approach. Ar3 and Ar4", J. Chem. Phys, 92 2481-87 (1990).
45. R. Moszynski, S. Rybak, S.M. Cybulski, G. Chalasinski, "Correlation Correction to the Hartree-Fock Electrostatic Energy Including Orbital Relaxation", Chem. Phys. Lett., 166 609-614 (1990).
46. M. M. Szczesniak, G. Chalasinski, S. M. Cybulski, S. Scheiner, "Intermolecular Potential of the Methane Dimer and Trimer", J.Chem. Phys. 93 4243-4253 (1990).
47. G. Chalasinski, M.M. Szczesniak, P. Cieplak, S. Scheiner, "Ab initio Study of Intermolecular Potential of H2O Trimer", J. Chem. Phys. 94 2873 (1991).
48. G. Chalasinski, M.M. Szczesniak, S. Scheiner, "Ab initio Study of the Intermolecular Potential of Ar-H2O", J. Chem. Phys. 94 2807-2816 (1991).
49. G. Chalasinski, M.M. Szczesniak, B. Kukawska-Tarnawska, "Ab initio Study of Intermolecular Potential for Ar-HCl", J. Chem. Phys. 94 6677-6685 (1991)
50. M.M. Szczesniak, R.A. Kendall, G. Chalasinski, "Ab initio Study of Nonadditive Effects in the Trimer of Ammonia", J. Chem. Phys., 95 5169-5178 (1991).
51. G. Chalasinski, M.M. Szczesniak, "Structure and Energy of van der Waals Complexes from Ab initio Calculations", Croatica Chimica Acta 65, 17-27 (1992).
52. M.M. Szczesniak, G. Chalasinski, S.M. Cybulski, "Analysis of Intermolecular Potential of Ar-CH4: An ab initio Study", J.Chem. Phys., 96 463 (1992).
53. Z. Latajka, S. Scheiner, G. Chalasinski "Basis Set Superposition Error in Proton Transfer Potentials", Chem. Phys. Lett. 196, 384-389 (1992).
54. M.M. Szczesniak, G. Chalasinski "Ab initio Calculations of Nonadditive Effects", Theochem 261, 37-54 (1992).
55. S.M. Cybulski, G. Chalasinski "Perturbation Analysis of the Supermolecular Interaction Energy and Basis Set Superposition Error" Chem. Phys. Lett, 197, 591-598 (1992).
56. G. Chalasinski, M.M. Szczesniak, S. Scheiner "Proton-Donor Properties of Water and Ammonia in van der Waals Complexes with Rare Gas Atoms. Kr-H2O and Kr-NH3", J. Chem. Phys. 97, 8181-8187 (1992).

57. M.M. Szczesniak, G. Chalasinski, S. Cybulski, P. Cieplak "Ab initio Study of the Potential Energy Surface of CH4-H2O", J. Chem. Phys. 98, 3078-3089 (1993).
58. G. Chalasinski, M.M. Szczesniak, S. Scheiner "Proton-Donor Properties of Water and Ammonia in van der Waals Complexes with Rare Gas Atoms. Be-H2O and Be-NH3", J. Chem. Phys. 98, 7020-7028 (1993)
59. J. Sadlej, G. Chalasinski, M.M. Szczesniak "On the Nature of the Interaction Energy in Ar-ClF Complex", J. Chem. Phys. 99, 3700-3705 (1993)
60. M. Gutowski, G. Chalasinski "Critical Evaluation of of Some Computational Approaches to the Problem of Basis Set Superposition Error", J. Chem. Phys. 98, 5540-5553 (1993).
61. R. Moszynski, S.M. Cybulski, G. Chalasinski "Many-Body Theory of Intermolecular Induction Interactions", J. Chem Phys. 100, 4998-5010 (1994)
62. B. Kukawska-Tarnawska, G. Chalasinski, M.M. Szczesniak "Helium Atom as a Probe of Molecular Shape and Properties. HeH2O Complex", Theochem 297, 313-325 (1993).
63. M.M. Szczesniak G. Chalasinski, P. Piecuch "The Nonadditive Interactions in the Ar2HF and Ar2HCl Clusters. Ab Initio Study" J. Chem. Phys. 99, 6732-6741 (1993).
64. J. Sadlej, G. Chalasinski, M.M. Szczesniak "On the Nature of the Interaction in the Ar-Cl2 Complex" Theochem 307, 187-199 (1994).
65. J. Sadlej, M.M. Szczesniak, G. Chalasinski "Ab initio Study of Ar-H2CO Complex" J. Chem. Phys. 99, 5211-5218 (1993).
66. G. Chalasinski, M.M. Szczesniak, R.A. Kendall "Supermolecular Approach to Many-Body Dispersion Interactions in Weak van der Waals Complexes. He, Ne, and Ar Trimers", J. Chem. Phys. 101, 8860-8869 (1994).
67. G. Chalasinski, M.M. Szczesniak "Origins of Structure and Energetics of van der Waals Clusters from Ab Initio Calculations." Chem. Rev. 94, 1723-1765 (1994).
68. B. Kukawska-Tarnawska, G. Chalasinski, K. Olszewski, "Structure and Energetics of van der Waals Complexes of Carbon Monoxide with Rare Gases. He-CO and Ar-CO", J. Chem. Phys. 101, 4964-4974 (1994).
69. G. Chalasinski, M. Gutowski, M.M. Szczesniak, J. Sadlej, S. Scheiner "Ab initio Study of He(1S) + Cl2(X1Sg,3Pu) Potential Energy Surfaces"J. Chem. Phys., 101, 6800-6809 (1994).
70. S.M. Cybulski, M.M. Szczesniak, G. Chalasinski "Ab initio Study of Nonadditive Interactions in Ar2HF and Ar2HCl.Part II. Analysis of Exchange and Induction Effects", J. Chem. Phys., 101,10708-10716 (1994).
71. M. Gutowski, M.M. Szczesniak, G. Chalasinski, "Comment on: "A Possible Definition of Basis Set Superposition Error"", Chem. Phys. Lett., 241, 140-145 (1995).
72. R. Burcl, S. M. Cybulski, M. M. Szczesniak, and G. Chalasinski, "Towards An Analytical Three-Body Potential of Ar2Cl-", J. Chem. Phys., 103, 299-308 (1995).
73. R. Burcl, G. Chalasinski, R. Bukowski, and M.M. Szczesniak, "On the Role of Bond Functions in Interaction Energy Calculations. Ar-HCl, Ar-H2O, (HF)2", J. Chem. Phys., 103, 1498-1506 (1995).
74. S.M. Cybulski, R. Burcl, G. Chalasinski and M.M. Szczesniak "Partitioning of Interaction Energy in van der Waals Complexes Involving Excited State Species. The He(1S)+Cl2(B,3Pu) Interaction", J. Chem. Phys. 103,10116-10127 (1995).
75. A.J. Abkowicz, Z. Latajka, S. Scheiner, and G. Chalasinski "Site-site Function and Successive Reaction Counterpoise Calculation of Basis Set Superposition Error for Proton Transfer", Theochem 342,153-159(1995).
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89. M.M. Szczesniak, J. Rak, nad G. Chalasinski "Preliminary observations on the dependence of potential energy surfaces on intramolecular degrees of freedom", NATO Advanced Study Institute, Ed. by S.S. Xantheas, (Kluver, Amsterdam, 2000) pp. 70-79.
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92. J. Sadlej, J. Makarewicz, and G. Chalasinski "Ab initio study of energy, structure and dynamics of the water-carbon dioxide complex", J. Chem. Phys. 109, 3919-3927 (1998).
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