

# Szabados Ágnes teljes publikációs listája

## I. Tudományos közlemények

1. P. R. Surján, Á. Szabados: Damping of perturbation corrections in quasidegenerate situations, *J. Chem. Phys.* **104**, 3320-3324 (1996).  
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2. P. R. Surján, Á. Szabados: Damping in perturbation theory, *Acta Univ. Debreceniensis* **XXX/2**, 97-111 (1995).  
**impakt faktor: – független hivatkozások : 0**
3. P. R. Surján, Á. Szabados, F. Bogár, J. Ladik: Calculation of correlation-corrected band structures of polymers in the case of quasi-degeneracy, *Solid State Communications* **103**, 639-644 (1997).  
**impakt faktor: 1.38 független hivatkozások : 1**
4. P. R. Surján, Á. Szabados: Dyson-corrected orbital energies for the perturbative treatment of electron correlation, *Int. J. Quantum. Chem.* **69**, 713-719 (1998).  
**impakt faktor: 1.25 független hivatkozások : 0**
5. P. R. Surján, M. Kállay, Á. Szabados: Non-conventional partitioning of the many-body Hamiltonian for studying correlation effects, *Int. J. Quantum. Chem.* **70**, 571-581 (1998).  
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6. Gy. Schultz, Á. Szabados, Gy. Tarczay and K. Zauer: Molecular Structure of 1,2,4,5-Tetracyanobenzene from Gas-Phase Electron Diffraction and Theoretical Calculations, *Struct. Chem.*, **10**, 149-155 (1999).  
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8. P. R. Surján, Á. Szabados: Optimized partitioning in perturbation theory: comparison to related approaches, *J. Chem. Phys.* **112**, 4438-4446 (2000).  
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9. Zs. Szekeres, Á. Szabados, M. Kállay and P. R. Surján: On the "killer condition" in the equation-of-motion method: ionization potentials from multi-reference wave functions, *Phys. Chem. Chem. Phys.* **3**, 696-701 (2001).  
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10. Á. Szabados, X. Assfeld and P. R. Surján: Near-degeneracy corrections for second-order perturbation theory: comparison of two approaches, *Theor. Chem. Acc.*, **105**, 408-412 (2001).  
**impakt faktor: 1.28 független hivatkozások : 0**
11. J. Noga, Á. Szabados and P. R. Surján: On the Use of Connected Moments Expansion with Coupled Cluster Reference, *Int. J. Mol. Sci.*, **3**, 508-521, (2002).  
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12. P. R. Surján, Á. Szabados: Constant Denominator Perturbative Schemes and the Partitioning Technique, *Int. J. Quantum. Chem.*, **90**, 20-26 (2002).  
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13. P. R. Surján, Á. Szabados and Zs. Szekeres: Nonsymmetric Perturbation Theory for improving Coupled Cluster wave functions, *Int. J. Quantum. Chem.*, **90**, 1309-1320 (2002).  
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14. Á. Szabados, P. R. Surján: Optimized partitioning in PT: application for the equation of motion describing ionization processes, *Int. J. Quantum. Chem.*, **92**, 160-167 (2003).  
**impakt faktor: 1.25 független hivatkozások : 0**
15. P. R. Surján, D. Kóhalmi and Á. Szabados: Optimized quasiparticle energies in many-body perturbation theory, *Coll. Czech. Chem. Comm.*, **68**, 331-339 (2003).  
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16. Á. Szabados and M. Hargittai: Molecular Structure of Carbene Analogues: A Computational Study, *J. Phys. Chem. A*, **107**, 4314-4321 (2003).  
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17. Z. Rolik, Á. Szabados and P. R. Surján: On the perturbation of multiconfiguration wave functions, *J. Chem. Phys.*, **119**, 1922-1928, (2003).  
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18. P. R. Surján, A. Lázár and Á. Szabados: Laplace-transformed denominators in perturbation theory: Linear-scaling second order treatment of weakly interacting nanostructures, *Phys. Rev. A.*, **68**, 062503 (2003).

**impakt faktor: 2.81 független hivatkozások : 0**

19. P. R. Surján and Á. Szabados: Convergence enhancement in perturbation theory, *Coll. Czech. Chem. Comm.*, **69**, 105-120 (2004).

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20. P. R. Surján, Z. Rolik, Á. Szabados and D. Kóhalmi: Partitioning in multi-configuration perturbation theory, *Ann. Phys. (Leipzig)*, **13**, 223-231 (2004).

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21. Á. Szabados and P. R. Surján: On the size-dependence of Feenberg scaling, *Int. J. Quant. Chem.*, *submitted*

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## II. Könyvfejezet

P. R. Surján and Á. Szabados: Appendix to "Studies in Perturbation Theory": the problem of partitioning, in: *Fundamental World of Quantum Chemistry: A Tribute to the Memory of Per-Olov Löwdin*, editors: E. J. Brändas and E. S. Kryachko, Kluwer, Dordrecht, (2004), *in press*

## III. Poszterek és előadások

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2. P.R.Surján and Á.Szabados, Damping of Perturbation Corrections in Quasidegenerate Situations, *WATOC 4th World Congress, Jerusalem, Israel, 7-12 July, 1996*. (poszter)
3. Á.Szabados and M.Kállay, Program Wicky: a general algorithm for evaluating second quantized matrix elements, *MATH/CHEM/COMP '97, Dubrovnik, Croatia, 1997*. (előadás)
4. P.R.Surján and Á.Szabados, Green's functions in quantum chemistry, *Université de Nancy, France, 1997*. (szeminárium)

5. P.R.Surján, M.Kállay and Á.Szabados, Non-conventional partitioning of the many-body Hamiltonian for studying correlation effects, *Sanibel Symposium, USA, 1998*. (poszter)
6. Á.Szabados, Repartitioning by level shifts for describing correlation in molecules, *School and Research Workshop on Correlation in Atoms and Molecules, Debrecen 1998*. (előadás)
7. Szabados Á. és Surján P., A szinteltolás módszere a perturbációszámításban, *VIII. Anyagszerkezet-kutatási konferencia, MTA Anyagszerkezeti Munkabizottsága, Budapest, 1998 május 22.* (előadás)
8. P.R.Surján and Á.Szabados, Perturbational Calculation of Intermolecular Interaction Energies by Kapuy's Partitioning, *Internat. Seminar on Electronic Structure of Extended Systems, Dedicated to Prof. Ede Kapuy on His 70<sup>th</sup> Birthday, Szeged, 25-26 Sept., 1998*. (előadás)
9. P.R.Surján and Á.Szabados, How to partition the Hamiltonian in perturbation calculations - optimized level shifts for low order corrections, *Department of Physics, Theoretical Physics Division, Linkping University, Sweden, 28 May, 1999*. (szeminárium)
10. Á.Szabados and P.R.Surján, Optimized level shifts for a better partitioning in perturbative correlation calculations, *WATOC 5th World Congress, London, 1-6 Aug., 1999*. (poszter)
11. P.R.Surján and Á.Szabados, Optimized level shifts in perturbation theory, *Intern. Congr. Theor. Chem. Phys. (ICTCP), Mexico, Mexico City, 8-13 Nov., 1999*. (poszter)
12. Á.Szabados and P.R.Surján, Perturbative electron propagator approximation computed with level shifts for estimating ionization potentials, *3rd European Conference on Computational Chemistry, Budapest, 4-8 Sept., 2000*. (poszter)
13. P.R.Surján, Á.Szabados and D. Köhalmi, MODERN ASPECTS OF PERTURBATION THEORY, with special attention to convergence problems and the problem of quasi-degeneracy in quantum chemical applications *Symposium on Molecular Informatics and Combinatorial Quantum Chemistry, Collegium Budapest, 2001 19-21 Febr., 2001*. (előadás)
14. P.R.Surján and Á.Szabados, The Green operator in quantum chemistry, *School and Workshop in Quantum Chemistry, Debrecen, May 2001*. (előadás)
15. P.R.Surján, Á.Szabados and Edina Rosta, Recent Advances in Multi-reference Perturbation Theory, *School and Workshop in Quantum Chemistry, Debrecen, May 2001*. (előadás)

16. Á.Szabados, B.Réffy and M.Hargittai, Different Molecular Species in the Vapors of Chromium Dichloride, *Strength from Weakness: the 32nd crystallographic course at Erice, Italy, 23 May - 3 June, 2001*. (poszter)
17. Á.Szabados, B.Réffy and M.Hargittai, The Electron Diffraction Study of the Vapor of Chromium Dichloride, *9th European Symposium on Gas Electron Diffraction, Blaubeuren, Germany, 27 June - 1 July, 2001*. (poszter)
18. Á.Szabados and P.Surján, Optimizing level shift parameters in PT - with applications in Unsöld theory, *European Summerschool in Quantum Chemistry, Tjörnarp, Sweden, 19 Aug. -1 Sept., 2001*. (poszter)
19. Szabados Á., Green függvények a kvantumkémiában, Atom- és Molekulafizikus találkozók, 2001. Szept. 7., Debrecen (előadás)
20. P. R. Surján and Á. Szabados, MRPT and non-iterative corrections to CC wave functions, *Sanibel Conference, St. Augustine, Florida, February 2002*. (poszter)
21. Á. Szabados and P. R. Surján, Optimized partitioning in PT, applied to the equation of motion describing ionization, *Sanibel Conference, St. Augustine, Florida, February 2002*. (poszter)
22. P. R. Surján and Á. Szabados, The problem of partitioning in PT, *Laboratoire de Chimie Théorique, Université Luis Pasteur, Strasbourg, France, 8 July, 2002*. (szeminárium)
23. Péter R. Surján and Ágnes Szabados, Recent developments in MRPT, *4th International Congress on Theoretical Chemical Physics (ICTCP-IV), Marly-le-Roi, France, 9-16 July 2002*. (előadás)
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25. Á.Szabados, D. Kóhalmi and P.R. Surján, Optimized one-particle energies in an MP-type perturbation theory, *VII. European Workshop on Quantum Systems in Chemistry & Physics, Čašta Papiernička, Slovakia, 2002*. (előadás)
26. Péter R. Surján Z. Rolik and Ágnes Szabados, The problem of partitioning in multi-reference perturbation theory, *VII. European Workshop on Quantum Systems in Chemistry & Physics, Čašta Papiernička, Slovakia, 2002*. (előadás)
27. P.R. Surján, Z. Rolik, D. Kóhalmi and Á. Szabados, Multiconfiguration Perturbation Theory, *Symposium in Honour of István Mayer, MTA KKKI, Budapest, 12 April, 2003*. (előadás)

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29. Á.Szabados and P.R. Surján, Analysis of some EOM techniques describing ionization, *Pomeranian Quantum Chemistry and Physics Workshop, Pobierowo, Poland, May 22-25., 2003* (előadás)
30. R. Rolik, Á. Szabados and P.R. Surján, Test calculations with multi-configurational perturbation theory, *2<sup>nd</sup> Central European Symposium on Theoretical Chemistry, Nové Hradý, Czech Republic, Sept. 25-28., 2003.* (poszter)
31. Á.Szabados, A. Lázár and P.R. Surján, Perturbative treatment of interacting nanosystems: the role of Laplace-transformed denominators, *2<sup>nd</sup> Central European Symposium on Theoretical Chemistry, Nové Hradý, Czech Republic, Sept. 25-28., 2003.* (előadás)
32. P.R. Surján, Á. Szabados, D. Kóhalmi and Z. Rolik, Do we really need a multi-reference formalism to describe potential surfaces in coupled-cluster theory?, *2<sup>nd</sup> Central European Symposium on Theoretical Chemistry, Nové Hradý, Czech Republic, Sept. 25-28., 2003.* (előadás)
33. Péter R. Surján and Ágnes Szabados, Open Questions in Perturbation Theory: the Problem of Partitioning, *Department of Physical Chemistry, Indian Association for the Cultivation of Science, Kolkata, India, Febr. 9, 2004.* (szeminárium)
34. Á.Szabados and P.R. Surján, Theoretical treatment of nanotube-nanotube interactions, *Department of Physical Chemistry, Indian Association for the Cultivation of Science, Kolkata, India, Febr. 12, 2004.* (szeminárium)
35. Á.Szabados and P.R. Surján, Theoretical treatment of nanotube-nanotube interactions, *Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India, Febr. 19, 2004.* (szeminárium)