P.R.SURJÁN

lectures, seminars and posters

1978 – 2023

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— The language of the title is the language of the presentation —
— The name of speaker or presenter is underlined —
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1978

1. Surján P.R.: Optikai rotátorerősségszámítás MTA KKKI Elméleti Kémia Csoport szemináriuma, 1978 február (seminar)

2. P.R.Surján: Offdiagonal hypervirial relations and the semiempirical calculation of optical rotatory strength International Seminar on Quantum Chemistry, Visegrád, Hungary, september 1978 (talk)

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1980

1. Surján P.R.: Pirido-[1,2a]-pirimidinek optikai aktivitása
MTA Anyagszerkezeti Munkabizottság előadóülése, Mátrafüred
(talk)

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1981

1. Surján Péter: A molekulák optikai aktivitásának elmélete
Magyar Kémikusok Egyesülete, Fizikai Kémiai Osztály előadódélutánja, 1981 márc. 9.
(talk)

2. P.R.Surján: A linearized SCF approximation
International seminar on quantum chemistry, Smolenice, Czechoslovakia, May 1981
(talk)

3. P.R.Surján: Rotációs barrierek számítása Extended Hückel elméletben
MTA KKKI, Budapest
(seminar)

4. P.R.Surján: Through space and through bond interactions leading to interbond delocalizations
Microsymposium on Quantum Chemistry, Liblice, Czechoslovakia, 7-11 September 1981
(poster)

5. M.Kajtár, P.R.Surján, K.Simon, I.Hermecz and Z.Mészáros: Molecular structure and chiroptical properties of tetrahydro-pyrido[1,2a] pyrimidin-4-one derivatives

Symposium on steric effects in Biomolecules, October 5-8, 1981, Eger, Hungary
(poster)

6. P.R.Surján and G.Náray-Szabó: Conformational analysis of the Ser-195 side chain in α-chymotrypsin using localized molecular orbitals
Symposium on steric effects in Biomolecules, October 5–8, 1981, Eger, Hungary
(poster)

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1982

1. P.R.Surján, I.Mayer and G.Náray-Szabó: On the different kinds of delocalization corrections to Strictly localized Molecular Orbitals
International Seminar on Quantum Chemistry , August 1982, Győr, Hungary
(talk)

2. P.R.Surján: On the evaluation of transition energies
Univ. of Vienna, Inst. for Solid State Physics
(invited seminar)

3. P.R.Surján: Konformációanalízis lokalizált pályákkal MTA KKKI, Budapest
(seminar)

4. M.Kertész and P.R.Surján: Trapping of phase kinks in polyacethylene, Germany, 1982
(poster)

5. Conformational analysis in light of localization and delocalization
International Symposium on Theoretical Organic Chemistry August 30 – September 3, 1983, Dubrovnik, Yugoslavia
(poster)

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1984

1. P.R.Surján: Chemical bonds and interbond interactions
Faraday Symposium on Quantum Chemistry, Cambridge 1984 (poster)

2. Geometry effects on the electronic structure of conjugated systems
University of Vienna, Inst. Solid State Phys. December 14, 1984 (invited seminar)

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1985

1. P.R.Surján, Á.Vibók and H.Kuzmany
Electronic Structure of Polyenes containing chain defects
International Winterschool on the Electronic Structure of Polymers 2 February – 1 March 1985, Kirchberg in Tirol, Austria
(poster)

2. Surján P.
Geometria, konjugáció és elektronszerkezet összefüggése poliacetilénben
MTA anyagszerkezeti munkabizottság előadóülése 1985 március, Visegrád
(talk)

3. P.R.Surján, I.Mayer and I.Lukovits
Second quantization based theory for intermolecular interactions without basis set superposition error
Workshop on Quantum Chemistry, Harmonia/Bratislava, Czechoslovakia, March 2O/22 1985
(talk)

4. I.Lukovits, P.R.Surján and I.Mayer: Strictly localized geminals
Workshop on Quantum Chemistry, Harmonia/Bratislava, Czechoslovakia, March 2O/22 1985

5. Quasiparticle transformations and a theory of the chemical bond
Fourth School of Advanced Methods of Quantum Chemistry Bachotek (Torun), Poland, 27 – 31 May
(poster)

6. Quasiparticle transformations and the theory of the chemical bond
Ruder Boskovic Institute, Zagreb, Yugoslavia, 30 October
(invited seminar)

7. I.Mayer and P.R.Surján: BSSE-free PT for intermolecular interactions
World Congress on Quantum Chemistry, Montreal, Canada, 1985

8. P.R.Surján, G.Náray-Szabó, I.Mayer and I.Lukovits
A new method for conformation analysis and potential surface calculations in biological systems
Internat.Symp. on Steric Aspects of Biomolecular Interactions, 26 – 29 August, Sopron, Hungary
(poster)

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1986

1. Quasiparticle transformations in thee theory of the chemical bond
Inst.Solid State Physics, University of Wien, 15 January
(invited seminar)

2. Second Quantized Approach to Quantum Chemistry
(short course)
The University of Newfoundland, Dept. Chemistry, St.Johns, Canada, March – April

5. P.R.Surján
Accidental degeneracy in C_2 molecules?
Canadian Chemical Society Conference, June 1 – 4, Saskatoon, Canada
(poster)

6. P.R.Surján
Quasiparticle transformations and the theory of the chemical bond
Canadian Chemical Society Conference, Saskatoon, Canada, June 1986
(poster)

7. P.R.Surján
Intermolecular Interactions

Mount Sinai Medical School, New York, USA
(invited seminar)

8. P.R.Surján
Second Quantized Approach to Quantum Chemistry
(3 invited seminars)
Georgetown University, Dept. Chemistry, Washington D.C., USA, June 1986

9. P.R.Surján
BSSE- ree perturbation theory for intermolecular interactions
International seminal on quantum chemistry,
Szeged, Hungary, August 1986

10. P.R.Surján
Quantum Chemical Evaluation of Transition Energies
Inst.Solid State Physics, University of Wien, November 1986
(invited seminar)

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1987

1. P.R.Surján
Quasiparticle transformations and the theory of the chemical bond: intra- and intermolecular interactions
Consejo Superior, Madrid, April 1987
(invited seminar)

2. Optical activity of thioamides
M.Kajtár, J.G.Ángyán and P.R.Surján
World Congress on Theoretical Organic Chemistry Budapest, Hungary, 1987
(lecture)

3. R.A.Poirier, A.Yadav and P.R.Surján
A preliminary investigation of retinal analogs
World Congress on Theoretical Organic Chemistry Budapest, Hungary, 1987
(lecture)

4. J.Cioslowski, M.Kertész and P.R.Surján
Connected moments expansion calculations of the correlation energy in small molecules
World Congress on Theoretical Organic Chemistry Budapest, Hungary, 1987
(poster)

5. P.R.Surján, I.Mayer and R.A.Poirier
Second quantization and the Hellmann-Feynman theorem: A unified view on energy derivatives
World Congress on Theoretical Organic Chemistry Budapest, Hungary, 1987
(poster)

6. S.Kugler, P.R.Surján and G.Náray-Szabó
Theoretical estimation of static charge fluctuations in amorphous silicon
World Congress on Theoretical Organic Chemistry Budapest, Hungary, 1987
(poster)

7. J.Kürti, H.Kuzmany and P.R.Surján
Disorder and effective conjugation length in conjugated polymers

World Congress on Theoretical Organic Chemistry Budapest, Hungary, 1987
(poster)

8. A.Yadav, R.A.Poirier and P.R.Surján
Retinal analogs in the ^{3}B like state
World Congress on Theoretical Organic Chemistry Budapest, Hungary, 1987
(poster)

9. A.Yadav, R.A.Poirier and P.R.Surján
Energy, geometry and valence: the influence of sulfur d/orbital exponent
World Congress on Theoretical Organic Chemistry Budapest, Hungary, 1987
(poster)

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1988

1. P.R.Surján
Electron pair methods vs independent particle approximation
International Symposium on the Electronic Structure and Properties of Molecules and Crystals
August 29 – Sept 3, 1988, Cavtat, Yugoslavia
(invited plenary talk)

2. I.Mayer and P.R.Surján
Improved SCF theory for intermolecular interactions without BSSE
International Symposium on Quantum Chemistry, Jerusalem, 1988 Aug 21 – 25
(poster)

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1989

1. Surján P.
Általanositott Hückel módszerek alkalmazása
BME Fizikai Intézet szeminariuma

2. J.Kürti and P.R.Surján
A simple model for studying quinoidal-aromatic transitions
Internat.Winterschool on the electronic structure of polymers, Austria, Kirchberg, 1989

3. I.Mayer, A.Vibók and P.R.Surján
BSSE-free SCF methods for intermolecular interactions.
Sixth School of Advanced Methods of Quantum Chemistry, Bachotek, Poland, 4 – 9 June 1989

4. P.R.Surján
Quinoid-Aromatic Structure of poly-iso-thionaphtene
TOC at MUN Conference, St.Johns, Canada 1989 July
(lecture)

5. P.R.Surján

Ab initio perturbation theory for intermolecular interactions
TOC at MUN Conference, St.Johns, Canada, 1989 July
(invited plenary lecture)

6. I.Mayer and P.R.Surján
Application of the chemical Hamiltonian approach to the problem of intermolecular interactions
Sannibel Symposium, Florida, USA 1989
(poster)

7. Rendezetlen rendszerek kvantumkémiája
Surján P.
MKE előadás, Szeged 1989 november
(talk)

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1990

1. P.R.Surján
Másodkvantálás és a Hellmann–Feynman tétel
BME Fizikai Intézet Szemináriuma, Február 2.
(seminar)

2. P.R.Surján
Nonlinear Schrödinger Equations and Intermolecular Interactions
MATH/CHEM/COMP/90: International course and conference on the interface between mathematics, chemistry and computer science, Dubrovnik, Yugoslavia, 25 – 30 June 1990
(invited lecture)

3. P.R.Surján and I.Mayer
Second quantization and exchange perturbation theories
WATOC '90: The second world congress on theoretical organic chemistry, Toronto, Canada, 8 – 15 July, 1990
(invited special lecture)

4. P.R.Surján
Exchange perturbációs elmélet
BME Fizikai Intézet Szemináriuma, 1990 December
(seminar)

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1991

1. Surján Péter
A hipervalens kén elektronszerkezete
ELTE TTK Szerves Kémai Tanszék szemináriuma, június 4
(seminar)

2. Surján Péter
Kis gerjesztési energiájú konjugált polimerek tervezése
MTA Anyagszerkezeti Munkabizottság konferenciája, Budapest május 23 – 24
(talk)

3. J.Kürti, P.R.Surján and M.Kertész
Searching for low-band-gap polymers
International Conference on Optical Probes of Organic Polymers, Snowbird, Utah, USA, August 19-22, 1991
(poster)

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1992

1. Surján Péter
Elektronkorreláció és szupravezetés
BME Fizikai Intézet szemináriuma, 1992 június
(seminar)

2. P.R.Surján and K.Németh
Quinoid-aromatic competition as a tool for band structure design
Intern.Conf. on Synth.Metals, Göteborg, Sweden, Aug. 1992
(poster)

3. J.Kürti, P.R.Surján, M.Kertész and G.Frapper
Design of small-gap conjugated polymers
Intern.Conf. on Synth.Metals, Göteborg, Sweden, Aug. 1992
(poster)

4. Surján Péter és Ángyán János
Variációs torzulások megakadályozása pszeudopotenciálokkal
Gáspár Rezső Szimpózium, Debrecen, 1992 október
(invited talk)

5. Surján Péter
Szigorúan lokalizált geminálok MO bázisban
BME Fizikai Intézet szemináriuma, 1992 november 13
(seminar)

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1993

1. Surján Péter, Udvardi László és Németh Károly
Jahn-Teller torzulások gerjesztett C_{60} molekulákban
BME Fizikai Intézet szemináriuma, 1993 február
(seminar)

2. Surján Péter, Udvardi László és Németh Károly
Jahn-Teller distorted excited states in C_{60}
Internat.Winterschool on the electronic structure of novel materials, Austria, Kirchberg, 1993 march
(poster)

3. P.R.Surján
Jahn-Teller distorted excited states of fullerenes
Consejo Supreior de Inv.Cientificas, Madrid, June 1993
(seminar)

4. P.R.Surján

Electronic Sturcture Calculation by Perturbed Strictly Localized Geminals
1st Congress of the Intern.Society of Chemical Physics Girona, Catalunia, Spain, July 1993
(invited talk)

5. P. R. Surján, L. Udvardi, and K. Németh
Jahn-Teller distorted excited states of C_{60}
WATOC'93 World Congress, July 1993, Toyohashi, Japan
(poster)

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1994

1. Surján Péter, Udvardi László és Németh Károly
Internat.Winterschool on the electronic structure of novel materials, Austria, Kirchberg, 1994 March
(poster)

2. László Udvardi, J.Kürti and P.R.Surján
Internat.Winterschool on the electronic structure of novel materials, Austria, Kirchberg, 1994 March
(poster)

3. Surján Péter
A C_{60} molekula elektrongerjesztései
A Magyar Tudományos Akadémia Fizikai Tudományok Osztályának és Kémiai Tudományok Osztályának tudományos ülésszaka Budapest, 1994 május 6
(lecture)

4. P.R.Surján
Correlation-induced interactions between chemical bonds
Sattellite Conference on Electron Correlation, Smolenice (Slovakia), June 1994
(lecture)

5. K.Németh, L.Udvardi and P.R.Surján
Semiempirical Studies on the Excited States of Buckminsterfullerene
8th International Congress of Quantum Chemistry Prague 1994
(poster)

6. P.R.Surján and J.G.Ángyán
On the reliability of the point charge model
8th International Congress of Quantum Chemistry Prague 1994
(poster)

7. P.R.Surján
Spin-adapted reduced Hamiltonians in non-orthogonal basis
MATH/CHEM/COMP/90: International conference on the interface between mathematics, chemistry and computer science, Dubrovnik, Croatia, June 1994
(invited lecture)

8. L.Udvardi, K.Németh, P.R.Surján, J.Kürti and S.Pekker
Calculation of the UV/VIS spectra of $C_{60}H_{2n}$ (n=1,2,3)
Intern.Conf. on Synth.Metals, Söul, South Korea, Aug. 1994
(poster)

9. P.R.Surján

Quantum Chemical Approach to Novel Materials: Small-gap Polymers and Fullerenes
Biannial Congress of the Spanish Chemical Society, Vitoria, Spain, September 1994
(invited lecture)

10. P.R.Surján
A ponttöltés modell a kvantumkémiában
ELTE Elméleti Kémia Tanszék szemináriuma, okt. 19.

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1995

1. P.R.Surján
Electronic Excitations in Fullerenes
University of Stuttgart, Institue of Solid State Physics January, 1994
(invited seminar)

2. P.R.Surján and K.Németh
Sp^3 Carbons in fullerenes
Internat.Winterschool on the electronic structure of novel materials, Austria, Kirchberg, 1995 March
(talk)

3. P.R.Surján, L.Udvardi and K.Németh,
Excited states of the C_{60} dimer
Materials Research Society Spring Meeting, Symp. K. on Fullerenes, Strassbourg, France, May 1995
(talk)

4. P.R.Surján
Electronic sturcture of fullerenes
University of Nancy, CNRS Lab Chimie Theorique, Nancy, June 1995
(seminar)

5. P.R.Surján
Electronic structure of fullerenes
DKFZ, Dept.Molecular Biology, Heidelberg, Germany, June 1995
(seminar)

6. K.Németh and P.R.Surján
Interaction of benzene with rare gas atoms
Int.Conf. on Molecular Quantum Mechanics, Cambridge, 3–7 September 1995
(poster)

7. P.R.Surján
Learning second quantization in one hour
School and Workshop in Quantum Chemistry, Debrecen, October 1995
(invited seminar)

8. P.R.Surján
Second quantization for composite particles
School and Workshop in Quantum Chemistry, Debrecen, October 1995
(invited seminar)

9. P.R.Surján and Á.Szabados

Damping in perturbation theory — a quantum chemical applicatioon
School and Workshop in Quantum Chemistry, Debrecen, October 1995
(talk)

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1996

1. K.Németh, M.Kállay, P.R.Surján
On the stability of Jahn–Teller distorted states of C_{60} and smaller fullerenes
Internat.Winterschool on the electronic structure of novel materials, Austria, Kirchberg, 1996 March
(poster)

2. P.R.Surján, J.G.Ángyán, A.Lázár, K.Németh and L.P.Bíró
On the nature of the chemical bond between the monomeric units of the fullerene polymer
Internat.Winterschool on the electronic structure of novel materials, Austria, Kirchberg, 1996 March
(poster)

3. R.R.Surján, L.Lain and C.Perez del Valle Second quantization based exchange perturbation theory – third order results for intermolecular interactions 2nd Congress of the Int.Soc.Theor.Chem.Phys., New Orleans, April 1996 (invited talk)

4. R.R.Surján, L.Lain and C.Perez del Valle Second quantization based exchange perturbation theory for intermolecular interactions Workshop on Electronic Structure of Complex Systems, Budapest, May 1996 (invited talk)

5. M.Kállay and P.R.Surján
Application of Group theory for Jahn-Teller Distorted Excited Fullerenes
Workshop on Electronic Structure of Complex Systems, Budapest, May 1996
(talk)

6. K.Németh and P.R.Surján
Zero-Field-Splitting of the Triplet States in C_{60} and in Thiophene oligomers
Workshop on Electronic Structure of Complex Systems, Budapest, May 1996
(talk)

7. P.R.Surján, K.Németh and M.Kállay Electronic Structure and Zero-Field-Splitting of C_{60} and other Fullerenes WATOC 4th World Congress, Jerusalem, Israel, July 7-12, 1996 (talk)

8. P.R.Surján and Á. Szabados Damping of Perturbation Corrections in Quasidegenerate Situations WATOC 4th World Congress, Jerusalem, Israel, July 7-12, 1996 (poster)

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1997

1. P.R.Surján, M.Kállay and Gy.Dömötör
Reaction coordinate analysis on the excited potential surface of fullerenes
Internat.Winterschool on the electronic structure of novel materials, Austria, Kirchberg, 1997 March

(poster)

2. P.R.Surján
Quantum chemistry of excited states: Tamm-Dankoff approximation with geminal-type wave functions
MATH/CHEM/COMP/97: International conference on the interface between mathematics, chemistry and computer science, Dubrovnik, Croatia, June 1997
(talk)

3. M.Kállay and P.R.Surján
Triplet state characteristics of higher fullerenes and fullerene dimers
MATH/CHEM/COMP/97: International conference on the interface between mathematics, chemistry and computer science, Dubrovnik, Croatia, June 1997
(talk)

4. A.Lázár and P.R.Surján
On the nature of excitations in molecular dimers
MATH/CHEM/COMP/97: International conference on the interface between mathematics, chemistry and computer science, Dubrovnik, Croatia, June 1997
(poster)

5. P.R.Surján and Á.Szabados
Green's functions in quantum chemistry
University of Nancy, CNRS Lab Chimie Theorique, Nancy, November 1997
(seminar)

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1998

1. P.R.Surján, M.Kállay and Á.Szabados
Non-conventional partitioning of the many-body Hamiltonian for studying correlation effects
Sanibel Conference, St.Augustine, Florida, February 1998 (poster)

2. P.R.Surján and Zsolt Szekeres
Highly symmetruc borane clusters as fullerene analogs
Internat.Winterschool on the electronic structure of novel materials, Austria, Kirchberg, 1998 March
(poster)

3. Surján Péter, Kállay Mihály és Lázár Armand:
A polimerizálódó Buckminster-fullerén
VIII. Anyagszerkezet-kutatási konferencia, MTA Anyagszerkezeti Munkabizottsága, Budapest, 1998 május 22
(előadás)

4. Szabados Ágnes és Surján P.
A szinteltolás módszere a perturbációszámításban
VIII. Anyagszerkezet-kutatási konferencia, MTA Anyagszerkezeti Munkabizottsága, Budapest, 1998 május 22
(előadás)

5. Surján P.
Green's functions in quantum chemistry, I-IV. School and Workshop in Quantum Chemistry, Debrecen, May 1998

(course)

6. 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 70th Birthday, Szeged, 25-26 September, 1998
(invited talk)

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1999

1. 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, Linköping University, Sweden, May 28
(seminar)

2. Péter R. Surján, and Mihály Kállay
Excitation Energies from Geminal-type Wave Functions
WATOC 5th World Congress, London, Aug 1-6, 1999
(poster)

3. Mihály Kállay and Péter R. Surján,
Geminal-based CI Calculations
WATOC 5th World Congress, London, Aug 1-6, 1999
(poster)

4. Á. Szabados and Péter R. Surján
Optimized level shifts for a better partitioning in perturbative correlation calculations
WATOC 5th World Congress, London, Aug 1-6, 1999
(poster)

5. Péter R. Surján and Mihály Kállay,
Improving CISD with geminal-type reference states
University of Nancy, CNRS Lab Chimie Theorique, Nancy, October 1999
(seminar)

6. Péter R. Surján
The Contracted Schrödinger Equation: a tutorial
University of Nancy, CNRS Lab Chimie Theorique, Nancy, October 1999
(seminar)

7. Péter R. Surján, M.Kállay and E.Rosta
A CISD and an MP2 method with geminal type reference state Int.Congr.Theor.Phys.Chem. (ICTCP), Mexico, 8-13 November, 1999
(invited talk)

8. Péter R. Surján and Á. Szabados
Optimized level shifts in perturbation theory
Int.Congr.Theor.Phys.Chem. (ICTCP), Mexico, 8-13 November, 1999
(poster)

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2000

1. Péter R. Surján
Second Quantized Approach to Quantum Chemistry
University of Nancy, CNRS Lab Chimie Theorique, Nancy, Apr 25–28 2000
(course)

2. Péter R. Surján
On the killer condition in excited state quantum chemistry
Consejo Superior, Madrid, 4 May
(seminar)

3. Péter R. Surján
Using second quantization: on the killer condition in excited state quantum chemistry
University of Nancy, CNRS Lab Chimie Theorique, Nancy, May 16 2000
(seminar)

4. Edina Rosta, Péter R. Surján, János Ángyán
Chemical Potentials and Fukui Functions from Coupled Hartree-Fock Equations
Chemical Bonding: State of the Art in Conceptual Quantum Chemistry, 1-4 June 2000, La Colle sur Loup (France)
(poster)

5. Edina Rosta, Péter R. Surján, János Ángyán
Chemical Potentials and Fukui Functions from Coupled Hartree-Fock Equations
Internat. Conf. on Density Functional Theory and its Applications to materials, Antwerp, Belgium, June 8–10 2000 (poster)

6. Edina Rosta, Péter R. Surján
The interaction of chemical bonds investigated by geminal-type wavefunction
Int.Congr. Quantum.Chem., Mounton, France, June 2000
(poster)

7. P. R. Surján,
Excited and Ionized States of Large Molecules: an MR-CIS Approach
Third European Conference on Computational Chemistry (EUCO-CC3), Budapest, 4–8 September 2000
(invited talk)

8. M. Kállay and P. R. Surján,
Computing coupled cluster wave functions with arbitrary excitations. Convergence of the CC series
Third European Conference on Computational Chemistry (EUCO-CC3), Budapest, 4–8 September 2000
(poster)

9. E. Rosta and P. R. Surján,
The interaction of chemical bonds investigated by geminal-type wave function
Third European Conference on Computational Chemistry (EUCO-CC3), Budapest, 4–8 September 2000
(poster)

10. Á. Szabados and P. R. Surján,
Perturbative electron propagator approximation computed with level shifts for

estimating ionization potentials
Third European Conference on Computational Chemistry (EUCO-CC3), Budapest, 4–8 September 2000
(poster)

11. Zs. Szekeres and P. R. Surján,
Kiler condition in EOM: A new approach for EOM-IP and EOM-EA Calculations
Third European Conference on Computational Chemistry (EUCO-CC3), Budapest, 4–8 September 2000
(poster)

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2001

1. Peter R. Surján, Ágnes Szabados and Dora Kohalmi
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 February 19–21
(invited talk)

2. Péter R. Surján and Ágnes Szabados
The Green operator in quantum chemistry
School and Workshop in Quantum Chemistry, Debrecen, May 2001
(invited talk)

3. Péter R. Surján Ágnes Szabados and Edina Rosta
Recent Advances in Multi-reference Petrutbation Theory School and Workshop in Quantum Chemistry, Debrecen, May 2001
(invited talk)

4. Edina Rosta and Péter R. Surján
The interaction of chemical bonds investigated by geminal-type wave function
School and Workshop in Quantum Chemistry, Debrecen, May 2001
(poster)

5. Zsolt Szekeres and Péter R. Surján
Ionization energy calculations using approximate density matrices School and Workshop in Quantum Chemistry, Debrecen, May 2001
(poster)

6. Surján Péter
A perturbációszámítás modern problémái
Atom- és Molekulafizikus Találkozó, Debrecen, 2001. Szeptember 7-8 (elH oadás)

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2002

1. P. R. Surján and Á. Szabados
MRPT and non-iterative corrections to CC wave functions
Sanibel Conference, St.Augustine, Florida, February 2002
(poster)

2. Péter R. Surján and Ágnes Szabados
The problem of partitioning in PT
Inst.Chem., Univ. Strassbourg, France, July 2002
(invited seminar)

3. Péter R. Surján and Ágnes Szabados
Recent developments in MRPT
Int.Congr.Theor.Phys.Chem. (ICTCP), Marly le Roi, France, July 2002
(talk)

4. Edina Rosta and Péter R. Surján
Two-body zeroth order Hamiltonians in multi-reference perturbation theory
WATOC 2002 World Congress, Lugano, Switzerland, July 2002
(poster)

5. Péter R. Surján Z. Rolik and Ágnes Szabados
The problem of partitioning in multi-reference perturbation theory
Seveth European Workshop on Quantum Systems in Chemistry and Physics, Casta Papiernicka nr. Bratislava, Slovakia, 10-15 September, 2002
(talk)

6. Ágnes Szabados, Dóra Kőhalmi and Péter R. Surján
Optimized one-particle energies in an MP-type perturbation theory
Casta Papiernicka nr. Bratislava, Slovakia, 10-15 September, 2002
(talk)

7. Á.Szabados and P.R. Surján
Superoperators in Calculating Ionization Potentials by Perturbation Theory
1st Central European Symposium on Theoretical Chemistry, Zwettl, Austria, 2002.
(talk)

8. P.R. Surján and Zs. Szekeres
Direct determination of localized MOs: the extended Huzinaga equation
1st Central European Symposium on Theoretical Chemistry, Zwettl, Austria, 2002.
(talk)

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2003

1. P.R. Surján, Z. Rolik, D. Kőhalmi and Á. Szabados
Multiconfiguration Perturbation Theory
Symposium in Honour of István Mayer, MTA KKKI, April 12, 2003, Budapest
(talk)

2. Zs. Szekeres and P.R. Surján
Localised Molecular orbitals from the Huzinaga and Szász equations
Pomeranian Quantum Chemistry and Physics Workshop, Pobierowo, Poland, May 2003
(talk)

3. Á. Szabados and P.R. Surján
Excitation and ionization energies from superoperator theory
Pomeranian Quantum Chemistry and Physics Workshop, Pobierowo, Poland,

May 2003
(talk)

4. P.R. Surján
Open problems in perturbation theory Pomeranian Quantum Chemistry and Physics Workshop, Pobierowo, Poland, May 2003
(invited talk)

5. R. Rolik, Á. Szabados and P.R. Surján
Test calculations with multi-configurational perturbation theory
2nd Central European Conference on Theoretical Chemistry (CESCTC2003)
Nové Hrady (Czech Rebublik), Oct. 25–28, 2003
(poster)

6. D. Kőhalmi and P.R. Surján
Semiclassical treatment of atomcules
2nd Central European Conference on Theoretical Chemistry (CESCTC2003)
Nové Hrady (Czech Rebublik), Oct. 25–28, 2003
(poster)

7. Zs. Szekeres and P.R. Surján
Group functions by building block equations
2nd Central European Conference on Theoretical Chemistry (CESCTC2003)
Nové Hrady (Czech Rebublik), Oct. 25–28, 2003
(talk)

8. Á. Szabados and P.R. Surján
Perturbative treatment of interacting nanosystems: the role of Laplace-transformed denominators
2nd Central European Conference on Theoretical Chemistry (CESCTC2003)
Nové Hrady (Czech Rebublik), Oct. 25–28, 2003
(talk)

9. P.R. Surján, Á. Szabados, D. Kőhalmi and Z. Rolik
Do we really need a multi-reference formalism to describe potential surfaces in coupled-cluster theory?
2nd Central European Conference on Theoretical Chemistry (CESCTC2003)
Nové Hrady (Czech Republik), Oct. 25–28, 2003
(talk)

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2004

1. Péter R. Surján and Ágnes Szabados
Open Questions in Perturbation Theory: the Problem of Partitioning
Indian Association for the Cultivation of Science, Kolkata, India, February 2004
(seminar)

2. Ágnes Szabados and Péter R. Surján
Theoretical treatment of nanotube-nanotube interactions
Indian Association for the Cultivation of Science, Kolkata, India, February 2004
(seminar)

3. Ágnes Szabados and Péter R. Surján
Theoretical treatment of nanotube-nanotube interactions

Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India, February 2004
(seminar)

4. P.R. Surján
Van-e még új fizika a kvantumkémiában?
Ortvay kollokvium, ELTE Fizika Tanszékcsoport, 2004. március 4.
(seminar)

5. Péter R. Surján, Dóra Kőhalmi, Ágnes Szabados, Gábor Tóth, Zoltán Rolik and Zsolt Szekeres
The contracted Schrödinger equation and linear scaling methods
Pomeranian Quantum Chemistry and Physics Workshop, Pobierowo, Poland, May 2004
(invited talk)

6. Ágnes Szabados and Péter R. Surján
Size dependence of Feenberg's scaling
Pomeranian Quantum Chemistry and Physics Workshop, Pobierowo, Poland, May 2004
(talk)

7. D. Kőhalmi, Á. Szabados, G. Tóth, Zs. Szekeres and P. R. Surján,
Obtaining the density matrix in the one-body framework: a new iterative formula
3rd Central European Symposium on Theoretical Chemistry, 2004, Tihany, Hungary
(talk)

8. Z. Rolik, Á. Szabados and P. R. Surján,
An efficient multiconfigurational PT code
3rd Central European Symposium on Theoretical Chemistry, 2004, Tihany, Hungary
(talk)

9. Zs. Szekeres, P.G. Mezey and P. R. Surján,
Helical graphite: Halfway between graphite and helicenes
3rd Central European Symposium on Theoretical Chemistry, 2004, Tihany, Hungary
(poster)

10. P.R. Surján,
Excursions in the fields of perturbation theory and linear scaling,
Dept. Theoretical Physics, Technical University, Budapest, 2004 November
(seminar)

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2005

1. Á. Szabados, D. Kőhalmi and P. Surján
Theoretical Treatment of Nanotube-Nanotube Interactions
Hungarian Nanotechnology Symposium, Budapest, 21-22 March, 2005
(talk)

2. Surján P.,

Perturbációszámítás a kvantumkémiában,
Magyar Tudományos Akadémia, Fizikai Tudományok Osztálya "*Atom- és Molekulafizika Ma*" c. előadóülése, Budapest, 2005.04.05.
(talk)

3. Á. Szabados, V. Rassolov, and P. R. Surján,
Perturbation theory with CEPA-0 like second order: a novel way to perturb multi-configurational wave functions
Fifth Congress of the Int. Soc. Theor. Chem. Phys., New Orleans, USA, July 20 -26, 2005
(poster)

4. P. R. Surján, P. Szakács, D. Kőhalmi, Á. Szabados, Z. Rolik and Zs. Szekeres,
Diagonalization-free Energy Calculations: Hartree-Fock and Beyond
13th European Seminar on Compoutational Methods in Quantum Chemistry (Strasbourg Seminar)
(invited talk)

5. Á. Szabados, V. Rassolov, and P. R. Surján,
CEPA-0-like perturbation corrections to geminal wave functions
4th Central European Symposium on Theoretical Chemistry, 25-28 September 2005, Sachticky, Slovakia
(talk)

6. D. Kőhalmi and P. R. Surján,
On the optimization of Davidson's α-matrix in many-body perturbation theory,
4th Central European Symposium on Theoretical Chemistry, 25-28 September 2005, Sachticky, Slovakia (talk)

7. Z. Rolik and P. R. Surján,
Orbital-free calculation of the MP2 energy correction,
4th Central European Symposium on Theoretical Chemistry, 25-28 September 2005, Sachticky, Slovakia (poster)

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2006

1. P. R Surján, D. Kőhalmi, Z. Rolik and Á. Szabados
Idempotent density matrices: Hartree-Fock and correlated calculations without molecular orbitals
XIIth International Congress of Quantum Chemistry, May 21-26, 2006 Kyoto, Japan
(invited talk)

2. Á. Szabados and P. R Surján
Theoretical modeling of nanotube bundles
Material-oriented Quantum Chemistry, Satelitte to the XIIth International Congress of Quantum Chemistry, May 27-29, 2006, Osaka, Japan
(talk)

3. P. R Surján
Perturbation theory of single- and multi-configurational states: the problem of partitioning,
Division of Physical Chemistry, Dept. of Chemistry, School of Science and Engineering, Waseda Univ., May 30, 2006 , okyo, Japan
(invited seminar)

4. Á. Szabados and P. R Surján
Theoretical interpretation of Grimme's spin-component-scaled Møller-Plesset approach
5th Central European Symposium on Theoretical Chemistry 2006, Septemner 24-27, Zakopane, Poland
(talk)

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2007

1. P. R Surján and P. Szakács
Convergence, Chaos or Divergence: Stability Analysis of the Coupled-Cluster Equations
Recent Trends in Many-Body methods for Electronic Structure and Properties of Atoms and Molecules, January 11-13, Orissa, India
(invited talk)

2. P. R Surján, D. Kőhalmi, P. Szakács, Á. Szabados and Z. Rolik
Towards large biomolecules: Hartree-Fock calculations and beyond,
From molecular informatics to bioinformatics, International symposium, 2007 March 19-21, Institute for Advanced Study, Collegium Budapest, Hungary
(invited talk)

3. ZS. Szekeres, P. G. Mezey and P. R. Surján,
Diagonalization-free initial guess to SCF calculations for large molecules,
From molecular informatics to bioinformatics, International symposium, 2007 March 19-21, Institute for Advanced Study, Collegium Budapest, Hungary
(invited talk)

3. P. R. Surján, D. Kőhalmi, P. Szakacs, A. Szabados and Z. Rolik
How to obtain the correlation energy from the Hartree-Fock density matrix?
Molecular Quantum Mechanics: Analytic Gradients and Beyond, A Conference in Honor of Peter Pulay, May 29- June 3, 2007, Margitsziget, Budapest, Hungary
(invited poster)

4. P. R. Surján, P. Szakács, Á. Szabados and Z. Rolik
Convergence, Chaos or Divergence: Stability Analysis of Iterative Procedures in Quantum Chemistry
16th Canadian Symposium on Theoretical Chemistry, August 4 - 9, 2007, MUN, St. John's, NL Canada
(invited talk)

5. P. Szakács and P. R. Surján
Exact π-electron Hamiltonians for curved systems
6th Central European Symposium on Theoretical Chemistry 2007, September 23-26, Litschau, Austria
(poster)

6. Surján Péter
Kalandozások két tudomány határán: bemutatkozó előadás
Bolyai Kollégium, Budapest, 2007 október 4.

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2008

1. Kürti Jenő, Péter Szalay, Kamarás Katalin és Surján Péter
Teller Ede hatása a magyar molekulafizikai kutatásokra
Teller Ede Centenáriumi ülés, Magyar Tudományos Akadémia, Budapest, 2008. jan. 16. (invited talk)

2. P. Surján
Effective π-electron hamiltonian for small-radii nanotubes: novel interpretation of curvature-induced conductivity
"2008 Molecular Informatics and Bioinformatics Symposium", Collegium Budapest, 2008 March 27-29
(invited talk)

3. M. Kobayashi, Á. Szabados, P. Surján and H. Nakai
Simple perturbave correction to the APSG wavefunction,
"11th Theoretical Chemistry Symposium (2008)", May 22–24, Keio University, Yokohama, Japan.

4. Surján Péter
Antilla Chimiae - Intézeti Szeminárium
ELTE Kémiai Intézet, 2008.05.29, Budapest.

5. P. Surján
Bloch-equation-based exact effective π-electron Hamiltonians for curved systems
13th International Workshop "Quantum Systems in Chemistry and Physics" (QSCP-XIII), Lansing, Michigan, July 6th – 12th, 2008.
(invited talk)

6. Masato Kobayashi, Agnes Szabados, Peter Surjan, Hiromi Nakai
Multiconfiguration perturbation theory using generalized Møller-Plesset partitioning and its application to APSG reference function
ISCTCP-VI, Vancouver, Canada, July 2008 (poster)

7. Agnes Szabados, Peter Surjan
Intruder-free partitionoing in multiconfigurational PT
7th Central European Conference on Theoretical Chemistry (CESTC-2008)
Hejnice, (Czech Republik), Sept. 28 – Oct 1, 2008
(talk)

8. Peter Szakacs, Dorina Kocsis and Peter Surjan
Jahn-Teller distortions in Carbon nanotubes
7th Central European Conference on Theoretical Chemistry (CESTC-2008)
Hejnice, (Czech Republik), Sept. 28 – Oct 1, 2008
(poster)

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2009

1. Peter Surjan, Peter Szakacs and Dorina Kocsis
Jahn-Teller distortions in Carbon nanotubes
Current Trends in Theoretical Chemistry and Physics
Raman Center for Atomic, Molecular and Optical Sciences, Indian Association for the CUltivation of Science, Calcutta, January 3rd, 2009 (invited talk)

2. Peter Surjan, Agnes Szabados and Zoltan Rolik
Multi-configuration Perturbation Theory
Workshop 2009: Recent Advances in Efficient Correlation Methods
(DFG Priority Program "Modern and Universal First-Principles Methods for Many-electron Systems in Chemistry and Physics",
11-13 March 2009, Benzberg (Koln), Germany (invited talk)

3. Peter Szakacs and Peter Surjan
Zero-field splitting of excited carbon nanotubes
8th Central European Conference on Theoretical Chemistry (CESTC-2009)
Dobogoko (Hungary), Sept. 25–28, 2009
(poster)

4. Zoltan Rolik, A. Szabados and Peter Surjan
Fourth order implementation of Multipartitioning MBPT
8th Central European Conference on Theoretical Chemistry (CESTC-2009)
Dobogoko (Hungary), Sept. 25–28, 2009
(poster)

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2010

1. Péter Szakács, Péter R. Surján
Jahn-Teller distortion and zero-field-splitting in carbon nanotubes 9th Central European Conference on Theoretical Chemistry (CESTC-2010)
Novy Smokovec, High Tatras (Slovakia), Sept. 12–15, 2010
(talk)

2. Zoboki Tamás, Mayer István, Surján R. Péter
Electron Correlation Calculations with Strictly Localized Orbitals 9th Central European Conference on Theoretical Chemistry (CESTC-2010)
Novy Smokovec, High Tatras (Slovakia), Sept. 12–15, 2010
(talk)

3. Péter Jeszenszki, Ágnes Szabados, Péter R.Surján
Exact diagonalization of bosonic Hamiltonians
9th Central European Conference on Theoretical Chemistry (CESTC-2010)
Novy Smokovec, High Tatras (Slovakia), Sept. 12–15, 2010
(poster)

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2011

1. Peter R. Surjan
Multi-reference perturbation theories
2011. August 26., Nanjing University, Laboratory of Theoretical Material Chemistry (LTMC), China
(invited seminar)

2. Peter R. Surjan
Multi-reference perturbation theories
2011. August 28., Biejing University, College of Chemistry and Molecular Engineering, China
(invited seminar)

3. Peter R. Surjan and Peter Jeszenszki
Composite particles in chemistry: from geminals to modeling cold atoms
ISTCP-VII September 2-8, 2011 Waseda University, Tokyo, Japan
(invited talk)

4. Peter R. Surjan
Wonders in Science: Superatomic Orbitals, or Simple Group Theory?
RAMET-2011, 1-4 December 2011, Puri, Orissa, India
(invited talk)

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2012

1. Agnes Szabados, Zsuzsanna Toth, Tamás Zoboki and Peter R. Surján
Electronic transitions of molecular fragments obtained by the Frozen Localized MO scheme, 11th Central European Conference on Theoretical Chemistry (CESTC-2012), Maripfarr, Austria, 2 – 5 September, 2012
(poster)

2. Péter R. Nagy, Peter R. Surján and Ágnes Szabados
π-electron contribution to Vibrational Optical Activity intensities, 11th Central European Conference on Theoretical Chemistry (CESTC-2012), Maripfarr, Austria, 2 – 5 September, 2012
(poster)

3. Tamás Zoboki, Peter R. Surján and Ágnes Szabados
Coupled Cluster-type corrections to geminal wave functions Tamás Zoboki, Péter R. Surján, Ágnes Szabados 11th Central European Conference on Theoretical Chemistry (CESTC-2012), Mariapfarr, Austria, 2 – 5 September, 2012
(poster)

4. Peter R. Surján, Zs. Tóth, T. Zoboki, and Á. Szabados
"Electron correlation calculation on molecular fragments for ground and excited states: the use of frozen localized molecular orbitals", Workshop on "Electron Correlation Methods: Past, Presence, and Future", in honor of Ivan Hubač and Miro Urban, Bratislava, October 12-13, 2012.
(invited talk)

5. Tóth Zsuzsanna, Zoboki Tamás, Szabados Ágnes, Surján Péter
"Molekulafrag-mens UV-VIS átmeneteinek számítása fagyasztott lokalizált molekulapálya módszerrel", MTA Anyag- és Molekulaszerkezeti Munkabizottság, MTA Szervetlen és Fémorganikus Kémiai Munkabizottság előadóülése, Szedres, 2012. október 13 – 14
(előadás)

5. Jeszenszki Péter, Surján Péter, Szabados Ágnes
"Egy multireferenciás perturbációs módszer spin-adaptálásának buktatói ". MTA Anyag- és Molekulaszerkezeti Munkabizottság, MTA Szervetlen és Fémorganikus Kémiai Munkabizottság előadóülése, Szedres, 2012. október 13 – 14
(előadás)

6. Nagy Péter, Szabados Ágnes, Surján Péter
"π-elektronrendszer hozzájárulása a rezgési optikai aktivitás intenzitáshoz", MTA Anyag- és Molekulaszerkezeti Munkabizottság, MTA Szervetlen és Fémorganikus Kémiai Munkabizottság előadóülése, Szedres, 2012. október 13 – 14
(előadás)

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2013

1. Péter Jeszenszki, Péter R. Surján, Ágnes Szabados
Sensitivity analysis in state-specific multireference perturbation theory
International Symposium on Theoretical Chemical Physics, Budapest, 25-31 August, 2013. (talk)

2. Péter R. Nagy, Péter R. Surján, Ágnes Szabados
Optical activity spectra of carbon nanostructures via a novel π-electron model
International Symposium on Theoretical Chemical Physics, Budapest, 25-31 August, 2013. (poster)

3. Tamás Zoboki, Ágnes Szabados, Péter R. Surján
Linearized Coupled Cluster Corrections to Antisymmetrized Product of Strongly Orthogonal Geminals: role of dispersive interactions
International Symposium on Theoretical Chemical Physics, Budapest, 25-31 August, 2013. (poster)

4. Szabados Ágnes, Zoboki Tamás és Surján Péter
Lokális spin stúdium: Az APSG hullámfüggvény és ennek perturbációs korrekciója
MTA Anyag- és Molekulaszerkezeti Munkabizottság előadóülése, Mátrafüred, 2013. október 17-19.

5. Surján Péter
Lokalizáció és delokalizáció: kémiai kötések kölcsönhatásai
MTA Anyag- és Molekulaszerkezeti Munkabizottság előadóülése, Mátrafüred,

2013. október 17-19.

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2014

1. Á. Szabados, T. Zoboki, P. Jeszenszi and P.R.Surján
Geminals with strong orthogonality - varieties, capabilities
16th European Seminar on Computational methods in Quantum Chemistry September 10-13 2014, Houffalize, Belgium
(invited talk)

2. Peter R. Surjan
Generalized Distributions to Describe Quasiclassical Mechanics
LUEST in TELLURIDE, Telluride Science Research Center, USA, 2014
(invited talk)

3. Á. Szabados, T. Zoboki, P. Jeszenszi and P.R.Surján
Geminals with strong orthogonality - varieties, capabilities
Central European Symposium on Theoretical Chemistry, 21-25. September 2014, Nagybörzsöny, Hungary
(talk)

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2015

1. P. R Surján, Zs. Mi'alka and Á. Szabados
Struggling with reference states in multi-reference theory
Recent Advances in Electronic Structure Theory , June 1-6, Nanjing, China
(invited talk)

2. Á. Szabados, P.R.Surján and P. Jeszenszi
Sypn-syummetry and size-consistency of strongly orthogonal geminals
Recent Advances in Electronic Structure Theory , June 1-6, Nanjing, China
(poster)

3. Péter R. Surján and Zs. Mihálka
Struggling with reference states in multi-reference theory
Symposium in Honor of J. Paldus
November 27, Praqgue, Czeh Republik
(invited talk)

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2016

1. Péter R. Surján, Zs. Mihálka and A. Szabados
Convergence enhancement in Rayleigh-Schrodinger Perturbation Theory: Quantum Chemical Applications
ISTCP-VIII July, July 17-22, 2016 Grand Forks, ND - USA
(invited talk)

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2017

1. Zsuzsanna É. Mihálka, Péter R. Surján
Dissociation potential curves from single reference Møller-Plesset PT
15th Central European Symposium on Theoretical Chemistry Wisła, Poland, September 3-6, 2017 (talk)

2. Péter Surján
The problem of convergence in perturbation theory
BME Elméleti Fizika Tanszék szemináriuma 2018. december 8.
(seminar)

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2018

1. Surján Péter
Divergens perturbációs sorok felösszegzéséről
SZEGED, Elméleti Fzikai Tanszék szemináriuma
2018 Február 22.
(seminar)

2. P.R. Surjan, Zs.E. Mihalka and A. Szabados
Large Order Perturbation Theory, Convergence Issues, Resummation and Extrapolation of Low-order Results
7th Japaneese-Czech Symposium on Qunatum Chemistry, Prague, May 21-24, 2018
(invited talk)

3. Geminal PT based on the UHF wavefunction
A. Szabados, D. Földvári, Zs. Tóth and P. R. Surján
16th Central European Symposium on Theoretical Chemistry Srni, Czech Republik, September 9–12
(talk)

4. Ádam Margocsy, Piotr Kowalski, Katarzyna Pernal,PéterSurjan, Ágnes Szabados
Multiple bond breaking with APSG based correlation methods
16th Central European Symposium on Theoretical Chemistry Srni, Czech Republik, September 9–12
(talk)

5. Zs. É. Mihálka, Peter R. Surján, Ágnes Szabados
Convergence issues in Rayleigh-Schrödinger Perturbation Theory – The inverse boundary value problem
16th Central European Symposium on Theoretical Chemistry Srni, Czech Republik, September 9–12
(poster)

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2019

1. Surján, Péter, Mihálka Éva Zsuzsanna, Szabados Ágnes
Divergens perturbációs sorok felösszegzése
Anyagtudományi Kiválósági Program Konferencia
Visegrád, 2019.január 14–16.
(talk)

2. Mihálka Éva Zsuzsanna, Szabados Ágnes, Surján, Péter,
Half-projection applied to the strongly orthogonal geminal product wavefunction
16th Central European Symposium on Theoretical Chemistry, 9th - 12th September 2019, Stadtschlaining, Austria
(talk)

3. Surján Péter
A γ függvény: gy új szemiklasszikus mechanika felé
MTA Anyag- és Molekulaszerkezeti Bizottság előadóülése,
Mátrafüred, 2019 október 11–12
(talk)

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2020

1. Margócsy Ádám, Surján P. és Szabados Á, Újabb eredmények a Coupled Cluster módszer geminál alapú általánosításában,
Anyagtudományi Kiválósági Program Konferencia
Visegrád, 2020.január 21–23.
(talk)

2. Mihálka Éva Zsuzsanna, Szabados Á. és Surján P., Spinsértő hullámfüggvények tisztítása (fél)projekciós technikával,
Anyagtudományi Kiválósági Program Konferencia
Visegrád, 2020.január 21–23.
(talk)

3. P. R. Surján
Coping with Divergent Perturbation Series,
University of Technology of Budapest, Faculty of Science, Institute of Mathematics,
Farkas Miklós Seminar, March 5, 2020
(seminar)

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2021

There were no conferences nor seminars due to the Covid pandemia this year.

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2022

1. P. R. Surján, Á. Szabados.
Many-body Perturbation Theory with Noncanonical Orbitals – a General Framework,
QSCP 2020 – 25th International Workshop on Quantum Systems in Chemistry, Physics and Biology,
19 – 24 June 2022, Toruń, Poland
(invited lecture)

2. Á. Szabados,Zs. E. Mihálka and P. R. Surján,
Perturbative Correction of Spin-unrestricted gemial wave functions with half-projections,
QSCP 2022 – 25th International Workshop on Quantum Systems in Chemistry, Physics and Biology,
19 – 24 June 2022, Toruń, Poland
(invited lecture)

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2023

1. Á. Szabados, Zs.E. Mihálka and P. R. Surján,
Spin-violating geminal wave functions and their correction by perturbation theory
ICQC 2023, Satellite Meeting on Strong Correlation in Molecules, 20 - 23th June Znojmo, Czech Republik
(invited lecture)

2. András Gombás, Zsuzsanna É. Mihálka, Ágnes Szabados, Péter Burlacu, and Péter R. Surján
To which extent can strong correlation be treated by single reference perturbation theory?
ICQC 2023, Satellite Meeting on Strong Correlation in Molecules, 20 - 23th June Znojmo, Czech Republik
(talk)

3. András Gombás, Ágnes Szabados and Péter Surján
Perturbation-adapted Perturbation Theory: Towards a Multi-Reference Approach,
MTA Anyag- és Molekulaszerkezeti Bizottság előadóülése,
Mátrafüred, 2023 november 24–25
(talk)

4. Surján Péter, Szabados Ágnes, Gombás András
A Davidson technika: egy kevéssé ismert eszköz
MTA Anyag- és Molekulaszerkezeti Bizottság előadóülése,
Mátrafüred, 2023 november 24–25
(talk)

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