6.1～6.30（7.1帰国）



**CURRICULUM VITAE OF** **2016 September 28**
**Prof. Paul G. Mezey**

## 1. PERSONAL:

Professor of Chemistry
Canada Research Chair in Scientific Modeling and Simulation,
Editor, Journal of Mathematical Chemistry,
Department of Chemistry and
Department of Physics and Physical Oceanography,
Memorial University of Newfoundland
283 Prince Philip Drive
St. John's, NL, A1B 3X7
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email: pmezey@mun.ca
Preferred email2: paul.mezey@gmail.com
http://www.mun.ca/research/chairs/mezey.php

Also:

Guest Professor of Chemistry ("Magantanar")
Institute of Chemistry
Eötvös University of Budapest
Budapest, Hungary
Tel. 00 36 30 25 30 820
Email : paul.mezey@gmail.com

Also :

Guest Professor
Faculty of Chemistry and Chemical Engineering,
Babes-Bolyai University, Cluj-Napoca, ROMANIA

Born in Nagyvarad, Hungary, Canadian Citizen and Hungarian Citizen

## 2. ACADEMIC CREDENTIALS:

| | | |
|---|---|---|
| M.Sc., Chemistry | University of Budapest, | 1967 |
| Ph.D., Chemistry (Summa Cum Laude, orig. dr.rer.nat), | University of Budapest, | 1970 |
| M.Sc., Mathematics (Distinction) | University of Budapest, | 1972 |
| D.Sc., Mathematical Chemistry (Distinction) | University of Saskatchewan, | 1985 |

## 3. APPOINTMENTS

| | |
|---|---|
| Canada Research Chair in Scientific Modelling and Simulation, and Professor of Chemistry, Department of Chemistry, Memorial University of Newfoundland | 2003-cont. |
| Cross-appointed, Dept. Physics and Phys. Oceanography, Memorial Univ. of Newfoundland | 2003-cont. |
| Visiting Research Professor of Mathematical Chemistry, Institute of Chemistry, Eötvös University, Budapest, Hungary | 1990-cont. |
| Albert Szent-Györgyi Fellow, Visiting Professor, Eötvös Loránd University of Budapest | 2002-2003 |
| Visiting Professor, Babes-Bolyai University, Cluj-Napoca, Romania | 2004-cont. |
| Foreign Scientific Associate, Institute for Fundamental Chemistry, Kyoto, Japan, | 1992-2001 |
| Professor of Chemistry, Department of Chemistry, University of Saskatchewan | 1982-2003 |
| Professor of Mathematics (cross-appointment as an Associate Member), Department of Mathematics and Statistics, University of Saskatchewan | 1986-2003 |
| Director, Mathematical Chemistry Research Unit, University of Saskatchewan | 1989-2003 |
| Associate Professor of Chemistry, Department of Chemistry and Chemical Engineering, University of Saskatchewan | 1979-82 |
| Assistant Professor of Chemistry, Department of Chemistry and Chemical Engineering, University of Saskatchewan | 1977-79 |

Lecturer, Department of Chemistry, University of Toronto 1975
PDF, University of Toronto, Department of Chemistry, 1973-76
Scientific Associate, Eötvös Loránd University of Budapest,
MTA Peptide Chemistry Research Group, Hungary, 1969-73

## 4. AWARDS and HONOURS

Distinguished Research Professor Award by the Kyoto University, International Research Unit of Advanced Future Studies, and the Yukawa Institute for Theoretical Physics, Kyoto University, Japan, July 9 – Aug 8, 2016, concerning the research collaboration with Prof. Noriko Fujii, at the Research Reactor Institute of Kyoto University, Osaka 2016

Award of the Japanese Society for Cataract Research, on the occasion of the Conference of the Japanese Society for Cataract Research, Morioka, Japan, 2016 July 28-30, concerning the invited lecture, Paul G. Mezey, "When molecules of the eye turn into their mirror images and become misfits: Right hands in left gloves." 2016

Computational and Mathematical Methods in Science and Engineering Award,
given at the CMMSE Conference, Rota, Cadiz – Spain, July 6-10, 2015
European Society of Computational Methods in Sciences and Engineering Award 2009
ICCMSE2009 Award (Internat. Conf. Computational Methods in Sciences and Engineering) 2009
IMI Distinguished Lecture Award, Industrial Mathematics Institute
Department of Mathematics, University of South Carolina, USA, 2008
"Magan Professor" Award, Eotvos University of Budapest, 2007
Bolyai Award for Support of Hungarian Language University Education in Transylvania 2007
Albert Szent-Györgyi Award of the Republic of Hungary 2002
Pro Universitate et Scientia Award, World Council of Hungarian University Professors, Budapest, Hungary 2003
Member of the European Academy of Sciences, Arts, and Humanities (Paris, France) 1999
Fellow, Institute for Advanced Study, Collegium Budapest, 1999
Member of the Hungarian Academy of Sciences 1998
Dr. Habil., University of Budapest, 1997
University of Saskatchewan Students' Union Teaching Excellence Award, 1996
KAO Lecture Award, Japan Society for Promotion of Science and
Institute for Fundamental Chemistry, Kyoto, 1995
Japan Society for Promotion of Science Award and Lecture Series: 1987
P.G. Mezey, The IRC Approach to Reaction Topology, Institute of Molecular Science, Okazaki, Japan, 1987 January 26.
P.G. Mezey, Global Optimization Techniques with Multiple Processors, Institute of Molecular Science, Okazaki, Japan, 1987 January 29.
P.G. Mezey, Molecular Chirality and Knot Theoretical Polynomials, Institute of Molecular Science, Okazaki, Japan, 1987 January 29.
P.G. Mezey, Symmetry-Independent Group Theory of Molecular Shapes, Institute of Molecular Science, Okazaki, Japan, 1987 January 30.
P.G. Mezey, The Propagation Basis Set Error in Molecular Hartree-Fock Calculations, Institute of Molecular Science, Okazaki, Japan, 1987 January 30.
P.G. Mezey, Molecular Shape and Molecular Chirality, University of Hiroshima, Hiroshima, Japan, 1987 January 21.
P.G. Mezey, The Intrinsic Reaction Coordinate and Reaction Topology, Kyoto University, Division of Molecular Engineering, Kyoto, Japan, 1987 February 3.

## 5. PROFESSIONAL ACTIVITIES:

Editor in Chief, Journal:
Journal of Mathematical Chemistry, Springer 1990-cont.
Editor in Chief, Book Serials:
Understanding Chemical Reactivity, Spinger Book Serial 1993-cont.
Advances in Molecular Similarity, JAI Press Book Serial 1995-2000
Mathematical and Computational Chemistry, Springer Book Serial 1999-2004

Editorial Board Member, Journals:

| | |
|---|---|
| ChemText, Topical Editor of Theoretical Chemistry, | 2014- cont. |
| SIAM Journal on Discrete Mathematics (Associate Editor) | 2007-2010 |
| Journal of Computational Chemistry, Wiley, | 1981-1998 |
| Structural Chemistry, Kluwer, | 1999-2002 |
| Journal of Computational Methods in Sciences and Engineering (JCMSE) Cambridge Internat. Science Publ. Ltd, | 2000-cont. |
| Turkish Journal of Chemistry | 1999-cont. |
| Journal of Mathematical Chemistry, Baltzer, | 1986-90 |
| MATCH Communications in Mathematical and Computational Chemistry | 2005-2011 |
| Reports on Molecular Theory, CRC Press | 1989-1992 |
| Molecular Engineering, Kluwer | 1990-1996 |
| International Journal of Quantum Chemistry, Wiley, | 1990-1995 |
| International Journal of Teaching and Case Studies, Inderscience, | 2007-cont. |
| International Journal of Technology Enhanced Learning (Associate Editor) | 2008-cont. |
| International Journal of Digital Culture and Electronic Tourism | 2008-cont. |

Editorial Board Member, Book Serials:

| | |
|---|---|
| Mathematical Chemistry, CRC Press Book Serial (Associate Editor) | 1993-2000 |
| Progress in Theoretical Chemistry and Physics, Kluwer Book Serial | 2000-2005 |
| Mathematical Modeling, Kluwer Book Serial | 1999-2002 |

Member: NSERC Strategic Grants Selection Committee, Open Area/New Directions 1990-1993

Member: Expert Panel on Pesticide Testing, Council of Canadian Academies/Conseil des académies canadiennes, Ottawa, Canada 2009-2011

## 6. ART EXHIBITIONS:

Paul G. Mezey: "Exhibition of Molecular Art Images", connected to the Invited Plenary Lecture.,Paul G. Mezey, "TOPOLOGICAL BEAUTY AND MOLECULAR SHAPE ", at the XVIII Generative Art Conference, Venice, Italy, 2015 December 9-11

Paul G. Mezey: "BEAUTY BEYOND THE MICROSCOPE: SHAPE, BEAUTY, AND FUNCTIONALITY IN THE MOLECULAR WORLD", Exhibition of Molecular Art images, EuroScience Open Forum ESOF 2004, Symposium and Exhibition entitled "Molecules as Art?", Stockholm, Sweden, 2004 Aug. 25-28,

Paul G. Mezey: "MOLECULES ARE BEAUTIFUL: SHAPE, BEAUTY, AND FUNCTIONALITY IN THE MOLECULAR WORLD", Art exhibition, Institute for Advanced Study, Collegium Budapest, Hungary, Dec. 6, 2000 - Jan. 9, 2001.

## 7. PROFESSIONAL SOCIETIES:

European Academy of Sciences, Arts, and Humanities, Paris (Full Member)
Hungarian Academy of Sciences (Foreign Member)
CODATA (UNESCO/ICSU) International, Paris, France (Secretary General, 1998-2004)
National Committee for CODATA, Ottawa, Canada (Chairman)
Institute for Advanced Study, Collegium Budapest (Fellow 1999, External Faculty 2005-)
International Society for Molecular Art (President, 2004-)
World Association of Theoretical Organic Chemists (Vice President 1990-96)
Centre de Mecanique Ondulatoire Appliquee, Paris, France (Member of the Scientific Board)
International Society for Mathematical Chemistry, Galveston, USA
Honorary Member, European Society of Computational Methods in Sciences and Engineering (2009)
Vice-President, World Council of Hungarian University Professors, Budapest, Hungary (2003-)
(From 2010, under new name, International Society of Hungarian University Professors)
Molecular Graphics Society
International Society for Quantum Biology and Pharmacology
Inter-American Photochemical Society
New York Academy of Sciences

American Association for the Advancement of Science
Canadian Society for Chemistry
Association of Canadian Theoretical Chemists

## 8. THESES SUPERVISED

Zoltan Antal, Ph.D., 2014, "Molecular Fragment and Substituent Effect Studies of Styrene Derivatives by Electron Density Shape Analysis"
Csaba Szakacs, Ph.D., 2009, "A theoretical study of the structure, energy, and shape of novel boron-nitrogen helices"
Zsolt Szekeres, Ph.D., 2007, „Fragment Theories in Wavefunction and Density Matrix Representations" ( Co-supervised with Prof. Peter Surjan )
Peter Warburton, Ph.D., 2003, "Approximate Chirality Measures"
Peter Warburton, M. Sc., 1999, "Balanced Basis Sets for a Single-Atom Sized Fragment MEDLA Database and Toxicological QShAR Applications"
Qishi Du, Ph. D., 1998, "A Heuristic Molecular Lipophilicity Potential as a Tool in Pharmaceutical Drug Design"
Gerard Heal, M.Sc., 1998, "Electrostatic Potential Patterns on Isodensity Surfaces: Tools for Molecular Modeling".
Duane Walker, Ph.D., 1993. "Shape Characteristics of Electronic Isodensity Surfaces for Small Molecules".
Xincai Luo, Ph.D., 1992. "Theoretical Studies on 2D Surfaces".
Victoria Jammal, M.Sc., 1989. "Contour Surface Analysis and Shape Group Studies: Application to Small Molecules and Drug Design".
Charu Hungenahally, M.Sc.,1988. "Study of Molecular Surfaces and Molecular Volumes".
A. Bruno, M.Sc., 1981. "An Analysis of the Excited Electronic States and a Theoretical Study of the Thioenolization Process of Aliphatic Thiocarbonyls". (Co-supervised by R.P. Steer)
A. K. Kapur, Ph.D., 1979. "Ab Initio SCF-MO Calculations of the Potential Surfaces of Thiocarbonyls". (Co-supervised by R.P. Steer)

## 9. RESEARCH ACTIVITY

**Author or co-author of 419 publications** in refereed scientific journals and books (over 200 single author papers).
**Author of two books:**
Mezey, P. G**.** *Potential Energy Hypersurfaces;* Elsevier: Amsterdam, 1987 (538 + xii pages)
Mezey, P. G. *Shape in Chemistry: An Introduction to Molecular Shape and Topology;*
VCH: New York, 1993 (224 + xi pages)
**Editor or co-editor of six books:**
*New Developments in Molecular Chirality;* Mezey, P.G., Ed.; Kluwer: Dordrecht, 1991.
*Mathematical Modeling in Chemistry ;* Mezey, P. G., Ed.; VCH: New York, 1991.
*Advances in Molecular Similarity,* Vol. 1, Carbo-Dorca, R., and Mezey, P. G., Jai Press, New York, 1997.
*Advances in Molecular Similarity,* Vol. 2, Carbo-Dorca, R., and Mezey, P. G., Jai Press, New York, 1998.
*Electron, Spin, and Momentum Densities and Chemical Reactivity ;* Mezey, P. G., and Robertson, B., Eds.; Kluwer Academic, Dordrecht, The Netherland, 2000.
*Linear –Scaling Techniques in Computational Chemistry and Physics, Methods and Applications;* J. Leszczynski, R. Zalesny, M. Papadopoulos, and P. G. Mezey Eds., Springer, New York, 2011,

## 10. MOST SIGNIFICANT RESEARCH CONTRIBUTIONS:

1. A theorem on the holographic relations between electron densities of molecular parts and complete molecules:
P.G. Mezey: "The Holographic Electron Density Theorem and Quantum Similarity Measures", *Molec. Phys.,* **1999**, *96*, 169-178 [paper 301], and a special, chirality and symmetry-related corollary of this theorem, P.G. Mezey: "Generalized Chirality and Symmetry Deficiency", *J. Math. Chem.,* **1998**, *23,* 65-84 [paper 285].
A rigorous proof is given for an important property of molecular electron densities: any small, nonzero-volume

piece of a fuzzy, boundaryless electron density cloud of a molecule contains the complete information about the entire molecule. This is a strengthening of the Hohenberg-Kohn theorem (W. Kohn, Nobel Prize 1998) establishing the relation between the complete electron density and molecular properties. The implications of the new result are far-reaching: in principle, the electron density cloud about a single H atom of a DNA molecule contains the complete information about this DNA molecule, hence, in principle, it contains the information about the genetic code.

2. Following the rigorous Intrinsic Reaction Coordinate (IRC) approach of Fukui and Fukui and Tachibana, a detailed study of reactions and conformational changes is given using potential energy surfaces and their multidimensional topological properties:
P.G. Mezey: *Potential Energy Hypersurfaces,* (Elsevier, Amsterdam, 1987, 538 + xii pages)
This is the first book describing in detail a comprehensive, unified model of all conformational changes and chemical reactions for a given collection of atomic nuclei and electrons, in terms of potential energy hypersurfaces. The topological properties of this multidimensional energy function of internal coordinates lead to surprising shortcuts, imply a group theory of reaction mechanisms, and also dispel many earlier misconceptions.

3. Rigorous molecular shape analysis methods, with special focus on chirality:
P.G. Mezey: *Shape in Chemistry: An Introduction to Molecular Shape and Topology,* (VCH:New York, 1993, 224 + xi pages).
A systematic introduction to the quantum chemical treatment of molecular shape and chirality, three-dimensional shape codes, shape similarity measures, molecular complementarity measures, chirality measures, and various alternative approaches and applications to drug design are described, exploiting the tools of modern mathematics, quantum chemistry and computer technology.
P.G. Mezey: "Quantum Chemistry of Macromolecular Shape", *Internat. Rev. Phys. Chem.* **1997,** *16,* 361-388 [paper 277].
The main new results are a new approach to the quantum chemical description of macromolecular electronic structure and a macromolecular electron density deformation method applicable to imitate the effects of small molecular distortions.
A special, chirality focus is found in:
P.G. Mezey (editor) "NEW DEVELOPMENTS IN MOLECULAR CHIRALITY", Kluwer, Dordrecht, 1991.

4. An efficient, *ab initio* quality linear-scaling macromolecular quantum chemistry method and computer programs have been developed, based on fuzzy molecular fragments:
The first version,
P.D. Walker and P.G. Mezey: "Ab initio Quality Electron Densities for Proteins: A MEDLA Approach" J. *Am. Chem. Soc.* **1994,** *116,* 12022-12032 [paper 244].
is the very first publication reporting *ab initio* quality electron densities and detailed images for proteins, at a resolution considerably exceeding x-ray crystallographic results; the first such result for any molecule beyond the one thousand atom limit.
A more advanced, density matrix based method is described in
P.G. Mezey: "Quantum Similarity Measures and Löwdin's Transform for Approximate Density Matrices and Macromolecular Forces", *Int. J. Quantum Chem.* **1997,** *63,* 39-48 [paper 263].
The main results are a new macromolecular similarity measure using new the ADMA (Adjustable Density Matrix Assembler) macromolecular quantum chemistry method, also used for the calculation of forces acting on various atoms in a macromolecule providing a new approach to the study of protein folding.

5. The quantum chemistry of molecular fragments and functional groups is placed on a new basis:
P.G. Mezey: "Functional Groups in Quantum Chemistry" *Adv. Quantum Chem.* **1996,** *27,* 163-222 [paper 259]
A systematic approach is developed for the quantum chemical study of functional groups.
P.G. Mezey, Fuzzy Electron Density Fragments in Macromolecular Quantum Chemistry, Combinatorial Quantum Chemistry, Functional Group Analysis, and Shape – Activity Relations, Accounts of Chem. Research, **47**, 2821-2827 (2014) , invited paper.

**11. EVIDENCE OF IMPACT:**

1. During the past one and a half decade, the Holographic Electron Density Theorem of Prof. Mezey has been employed by several independent research groups internationally, in Germany, Spain, Belgium, Japan, China, Russia, USA, Canada, as evidenced by their numerous publications.

2. A review of Prof. Mezey's book, "Shape in Chemistry: An Introduction to Molecular Shape and Topology" (VCH: New York, 1993) writes "Mezey is the most significant contributor to the discussion on molecular shape in the latter half of the twentieth century" (Angew. Chem., Int. Ed. Eng. **1993,** 34, 361).

3. Scientific contributions of Prof. Mezey and their impact have been reviewed on three occasions by Chemistry & Engineering News (C&EN), the official publication of the American Chemical Society: C&EN, May 9, 1983, p45; C&EN, Jan.22, 1990, p18; C&EN, Aug.14, 1995, p29.

4. In the past decade, over 120 invited lectures were given at international conferences, Universities and industry.

**LIST OF PUBLICATIONS** **2016 September 29**
**PAUL G. MEZEY**

**BOOKS:**

P.G. Mezey: " POTENTIAL ENERGY HYPERSURFACES "
Elsevier, Amsterdam, 1987. (538 + xii pages)

P.G. Mezey, (editor) "NEW DEVELOPMENTS IN MOLECULAR CHIRALITY"
Kluwer, Dordrecht, 1991. (294 + xii pages)

P.G. Mezey, (editor) "MATHEMATICAL MODELING IN CHEMISTRY"
VCH Publishers, New York, 1991. (386 + xii pages)

P.G. Mezey: "SHAPE IN CHEMISTRY: AN INTRODUCTION TO MOLECULAR SHAPE AND TOPOLOGY"
VCH Publishers, New York, 1993. (224 + xi pages)

P.G. Mezey B. Robertson, (editors) "ELECTRON, SPIN, AND MOMENTUM DENSITIES AND CHEMICAL REACTIVITY"
Kluwer Academic, Dordrecht, The Netherland, 2000.

R. Carbo-Dorca X. Girones, and P.G. Mezey (editors) "FUNDAMENTALS OF MOLECULAR SIMILARITY"
Kluwer Academic/Plenum Publ., New York, USA, 2001.

J. Leszczynski, R. Zalesny, M. Papadopoulos, and P. G. Mezey (editors) "LINEAR-SCALING TECHNIQUES IN COMPUTATIONAL CHEMISTRY AND PHYSICS, METHODS AND APPLICATIONS"
Springer, New York, 2011,

**JOURNAL PAPERS AND BOOK CHAPTERS**:

419. P. G. Mezey, How the Beauty of Concepts Becomes the Beauty of Shapes in Molecular Modelling. Invited paper, In: CroArtScia Conference Proceedings Series, Ruder Boskovic Institute Publ., Zagreb, Croatia (accepted May 2015).

418. P.G. Mezey, A Trigonometrically Scaled Multiple Tiling Approach For Error Reduction of Models Built From Fuzzy Fragments
Journal of Computational Methods in Sciences and Engineering (JCMSE),
in press, accepted 2016 Aug 3.

417. P.G. Mezey, Iterated Similarity Sequences and Factorial Level Similarities in Databases
Journal of Computational Methods in Sciences and Engineering (JCMSE),
in press, accepted 2016 Aug 3.

416. P.G. Mezey, On the Dimension Dependence of the Level of Optimality of Certain Multidimensional Sampling Strategies
Journal of Computational Methods in Sciences and Engineering (JCMSE),
in press, accepted 2016 Aug 3.

415. P. G. Mezey, Topological tools for the study of Families of Reaction Mechanisms: the Fundamental Groups of Potential Surfaces in the Universal Molecule Context. Chapter 9, In: Challenges and Advances in Computational Chemistry and Physics, Vol 22, "Applications of Topological Methods in Molecular Chemistry", Springer. Editors: Esmail Alikhani, Remi Chauvin, Christine Lepetit, and Bernard Silvi, DOI: 10.1007/978-3-319-29022-5_9 Challenges,Comp.Chem.,Phys., **22**, 243-255 (2016).

414. P. G. Mezey, Topological Beauty and Molecular Shape,
Conference Proceedings of the XVIII. Generative Art Conference, University of Milano Press, Milano, Italy, 2015, pages 256-259.
Available at http://www.generativeart.com/ga2015_WEB/topological-beauty_Mezey.pdf

413. P. G. Mezey, Decomposition and Fragmentation Principles in Computational Chemistry,
Proceedings of the International Conference on Computational Methods in Science and Engineering 2015 (ICCMSE 2015) , AIP (American Institute of Physics) Conference Proceedings,
doi: 10.1063/1.4938766 @ 2015 AIP Publishing LLC 978-0-7354-1349-8/$30.00
020002-1 – 020002-7

412. P. G. Mezey, Compensation Effects in Molecular Interactions and the Quantum Chemical le Chatelier Principle,
Invited paper to the Jacopo Tomasi Festschrift
J. Phys. Chem. A, **119**, 5305–5312 (2015).

411. P. G. Mezey: Relations Between Real Molecules Through Abstract Molecules: The Reference Cluster Approach
Invited paper , Theor. Chem. Accounts (Surjan Festschrift).
Theor. Chem. Acc. (2015) 134:134 DOI 10.1007/s00214-015-1728-1

410. P. G. Mezey, Alternative Algebraic Approaches in Quantum Chemistry, AIP (American Institute of Physics) Conference Proceedings, Vol. 1642, Proceedings of the International Conference on Computational Methods in Science and Engineering 2010 (ICCMSE 2010) AIP Conf. Proc. **1642**, 235-238 (2015).

409. P.G. Mezey, Fuzzy Electron Density Fragments in Macromolecular Quantum Chemistry, Combinatorial Quantum Chemistry, Functional Group Analysis, and Shape – Activity Relations, Accounts of Chem. Research, **47**, 2821-2827 (2014) , invited paper.

408. Z. Antal and P. G. Mezey, Substituent Effects and Local Molecular Shape Correlations,
Phys. Chem. Chem. Phys., **16**, 6666-6678 (2014).

407. Z. Antal, P. L. Warburton, and P. G. Mezey, Electron Density Shape Analysis of a Family of Through-Space and Through-Bond Interactions,
Phys. Chem. Chem. Phys., **16**, 918-924 (2014).

406. P.G. Mezey, Relations Between Nuclear Configuration Space and M-Space Symmetries of Chemical Reactions, (invited paper)
J. Internat. Soc. Interdisc. Study Symmetry, **2013**, 240-243 (2013).

405. P.G. Mezey, Molecular Modeling: An Open Invitation for Applied Mathematics,
AIP (American Institute of Physics) Conference Proceedings.,
DOI: 10.1063/1.4825416

404. P.G. Mezey, On the Inherited "Purity" of Certain Extrapolated Density Matrices, Computational and Theoretical Chemistry, **1003**, 130-133 (2013).

403. P.G. Mezey, Natural Molecular Fragments, Functional Groups, and Holographic Constraints on Electron Densities,
Phys. Chem. Chem. Phys., 14, 8516-8522 (2012).

402. E. Simon and P.G. Mezey,
Imperfect Periodicity and Systematic Changes of Some Structural Features Along Linear Polymers: The Case of Rod-Like Boron/Nitrogen Nanostructures,
Theor Chem Acc (2012) 131:1097
(honoring Prof. Akira Imamura, invited paper).
Published online 10 February 2012, DOI 10.1007/s00214-012-1097-y

401. P.G. Mezey,

Unexpected Expectation Values for Latent Molecular Properties,
J. Math. Chem., 50, 843-849 (2012).

400. Z. Antal and P.G. Mezey,
Molecular Fragment Shape Variation Index Applied to Intramolecular Interaction Studies,
J. Math. Chem., 50, 942-948 (2012).

399. E. Simon and P.G. Mezey,
Fragment Shape Variation Index for Periodicity Deficiency and Gradual Changes of Internal Coordinates Along Linear Polymers,
J. Math. Chem., 50, 934-941 (2012).

398. P.G. Mezey,
Molecular Fragment Shape Variation Index for Functional Groups and the Holographic Properties of Electron Density,
J. Math. Chem., 50, 926-933 (2012).

397. S. Arimoto, M. Spivakovsky, E. Yoshida, K. F. Taylor, and P. G. Mezey, Proof of the Fukui conjecture via resolution of singularities and related methods. V,
J. Math. Chem., 49, 1700-1712 (2011).

396. P.G. Mezey,
Chirality and Achirality Relations Along Reaction Paths, in "The Soai Reaction and Related Topics", Eds.: G. Palyi, C. Zucchi, and L. Caglioti, Artestampa - Accademia Nazionale di Scienze, Lettere ed Arti, Modena, 2012, pp 149-168.

395. P.G. Mezey, Fuzzy Electron Density Fragments as Building Blocks in Crystal Engineering Design in "The Importance of Pi-Interactions in Crystal Engineering (Frontiers in Crystal Engineering 3)", Eds. E. Tiekink and J. Zukerman-Schpector, John Wiley & Sons., New York, 2012, pp 233-241.

394. Zs. Szekeres and P.G. Mezey, Fragmentation Selection Strategies in Linear Scaling Methods, in "Linear-Scaling Techniques in Computational Chemistry and Physics, Methods and Applications", Eds. J. Leszczynski, R. Zalesny, M. Papadopoulos, and P. G. Mezey, Springer, New York, 2011, pp 147-156.

393. P.G. Mezey, Linear Scaling Methods Using Additive Fuzzy Density Fragmentation, in "Linear-Scaling Techniques in Computational Chemistry and Physics, Methods and Applications", Eds. J. Leszczynski, R. Zalesny, M. Papadopoulos, and P. G. Mezey, Springer, New York, 2011, pp 129-146.

392. P.G. Mezey, Computer Modeling of Herbicides and Pesticides in Environmental Regulations, in: "Proceedings of VII. Environmental Science Conference of the Carpathian Basin" Eds: I. Mócsy, K. Szacsvai, I. Urák, A. Zsigmond, A. Szikszai, Vol. I, pp. 51-55, Abel Publishers, Cluj, Romania), 2011, Vol. I., pp. 51-55.
(In Hungarian: Mezey Pál: Számítógépes modellezés a gyomírtószerek és rovarírtó szerek környezetvédelmi szabályozásában. In: Mócsy I., Szacsvai K., Urák I., Zsigmond A., Szikszai A. (szerk.), *VII. Kárpát-medencei környezettudományi konferencia*, I. kötet, Ábel Kiadó 2011, pp. 51-55)

391. S. Arimoto, M. Spivakovsky, K. F. Taylor, and P. G. Mezey, Proof of the Fukui conjecture via resolution of singularities and related methods. IV,
J. Math. Chem., **48**, 776-790 (2010).

390. C. Majdik, S. Burca, C. Indolean, A. Maicaneanu, M. Stanca, Sz. Tonk, and P.G. Mezey,
Suspended and Immobilized Brewery Waste Biomass and Commercial Yeast as Biosorbents for Cd(II) Removal. A Thermodynamic Study.
Rev. Roum. Chim., **55**(11-12), 871-877 (2010).

389. C.E. Szakacs and P.G. Mezey,
Laterally extended spiral graphite analogue boron-nitrogen helices,
J. Phys. Chem. A, **113**, 5157-5159 (2009).

388. P.G. Mezey,
Symmetry of Molecules On and Off Reaction Paths,
J. Internat. Soc. Interdisc. Study Symmetry, **2009**, 164-167 (2009).

387. P.G. Mezey,
Molecular Modeling and the Violation of Linear Scaling Principles,
AIP (American Institute of Physics) Conference Proceedings, Vol. 1504,
COMPUTATION IN MODERN SCIENCE AND ENGINEERING: Proceedings of the International Conference on Computational Methods in Science and Engineering 2009 (ICCMSE 2009): Volume 1504; pp. 43-49 (2012).

386. P.G. Mezey,
Discrete Skeletons of Continua in the Universal Molecule Model,
AIP (American Institute of Physics) Conference Proceedings, Vol. 1504,
COMPUTATION IN MODERN SCIENCE AND ENGINEERING: Proceedings of the International Conference on Computational Methods in Science and Engineering 2009 (ICCMSE 2009): Volume 1504; pp. 725-728 (2012).

385. P.G. Mezey,
Fundamental Constraints on Linear Scaling Methods: Relations between the Parts and the Whole in Molecules,
AIP (American Institute of Physics) Conference Proceedings, Vol. **1148**
COMPUTATION IN MODERN SCIENCE AND ENGINEERING: Proceedings of the International Conference on Computational Methods in Science and Engineering 2008 (ICCMSE 2008): Volume **1148**; pp. 669-673 (2009).

384. P.G. Mezey,
T-Hulls, Discretization, and Partially Ordered Sets in Molecular Shape Analysis,
AIP (American Institute of Physics) Conference Proceedings, Vol. **1148**
COMPUTATION IN MODERN SCIENCE AND ENGINEERING: Proceedings of the International Conference on Computational Methods in Science and Engineering 2008 (ICCMSE 2008): Volume **1148**; pp. 437-439 (2009).

383. P.G. Mezey,
Quantum Chemistry of Non-Bonded Interactions, Self-Avoiding Isodensity Contours and the Low Density Glue Bonding in Proteins,
Lecture Series on Computer and Computational Sciences, **7**, 1511-1514, (2006).

382. P.G. Mezey,
Size Measures of Molecular Electron Densities – From the Smith Measure of Electron Pairs to Local and Global Macromolecular Measures,
Lecture Series on Computer and Computational Sciences, **6**, 1-4, (2006).

381. C.E. Szakacs and P.G. Mezey,
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Extreme Values of Force Constants and Mean-Square Amplitudes of Vibration in Ethylene Type Molecules, I, $C_2H_4$ and $C_2D_4$,
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**RESEARCH FOCUS OF 2016 September 29**

**Prof. Paul G. Mezey**

## 1. HOLOGRAPHIC ELECTRON DENSITY THEOREM

A theorem on the holographic relations between electron densities of molecular parts and complete molecules:
P.G. Mezey: "The Holographic Electron Density Theorem and Quantum Similarity Measures", *Molec. Phys.,* **1999**, *96*, 169-178 [paper 301], and a special, chirality and symmetry-related corollary of this theorem, P.G. Mezey: "Generalized Chirality and Symmetry Deficiency", *J. Math. Chem.,* **1998**, *23,* 65-84 [paper 285].
A rigorous proof is given for an important property of molecular electron densities: any small, nonzero-volume piece of a fuzzy, boundaryless electron density cloud of a molecule contains the complete information about the entire molecule. This is a strengthening of the Hohenberg-Kohn theorem (W. Kohn, Nobel Prize 1998) establishing the relation between the complete electron density and molecular properties. The implications of the new result are far-reaching: in principle, the electron density cloud about a single H atom of a DNA molecule contains the complete information about this DNA molecule, hence, in principle, it contains the information about the genetic code.

## 2. THEORY OF POTENTIAL ENERGY SURFACES OF REACTIVE MOLECULES

Following the rigorous Intrinsic Reaction Coordinate (IRC) approach of Fukui and Fukui and Tachibana, a detailed study of reactions and conformational changes is given using potential energy surfaces and their multidimensional topological properties:
P.G. Mezey: *Potential Energy Hypersurfaces,* (Elsevier, Amsterdam, 1987, 538 + xii pages)
This is the first book describing in detail a comprehensive, unified model of all conformational changes and chemical reactions for a given collection of atomic nuclei and electrons, in terms of potential energy hypersurfaces. The topological properties of this multidimensional energy function of internal coordinates lead to surprising shortcuts, imply a group theory of reaction mechanisms, and also dispel many earlier misconceptions.

## 3. SHAPE-ANALYSIS OF MOLECULAR ELECTRON DENSITIES

Rigorous molecular shape analysis methods HAVE BEEN DEVELOPED, with special focus on chirality:
P.G. Mezey: *Shape in Chemistry: An Introduction to Molecular Shape and Topology,* (VCH:New York, 1993, 224 + xi pages).
A systematic introduction to the quantum chemical treatment of molecular shape and chirality, three-dimensional shape codes, shape similarity measures, molecular complementarity measures, chirality measures, and various alternative approaches and applications to drug design are described, exploiting the tools of modern mathematics, quantum chemistry and computer technology.
P.G. Mezey: "Quantum Chemistry of Macromolecular Shape", *Internat. Rev. Phys. Chem.* **1997,** *16,* 361-388 [paper 277].
The main new results are a new approach to the quantum chemical description of macromolecular electronic structure and a macromolecular electron density deformation method applicable to imitate the effects of small molecular distortions.
A special, chirality focus is found in:
P.G. Mezey (editor) "NEW DEVELOPMENTS IN MOLECULAR CHIRALITY", Kluwer, Dordrecht, 1991.

## 4. MACROMOLECULAR QUANTUM CHEMISTRY SOFTWARE

An efficient, *ab initio* quality linear-scaling macromolecular quantum chemistry method and computer programs have been developed, based on fuzzy molecular fragments:
The first version,
P.D. Walker and P.G. Mezey: "Ab initio Quality Electron Densities for Proteins: A MEDLA Approach" J. *Am. Chem. Soc.* **1994,** *116,* 12022-12032 [paper 244].
is the very first publication reporting *ab initio* quality electron densities and detailed images for proteins, at a resolution considerably exceeding x-ray crystallographic results; the first such result for any molecule beyond the one thousand atom limit.
A more advanced, density matrix based method is described in
P.G. Mezey: "Quantum Similarity Measures and Löwdin's Transform for Approximate Density Matrices and Macromolecular Forces", *Int. J. Quantum Chem.* **1997,** *63,* 39-48 [paper 263].

The main results are a new macromolecular similarity measure using new the ADMA (Adjustable Density Matrix Assembler) macromolecular quantum chemistry method, also used for the calculation of forces acting on various atoms in a macromolecule providing a new approach to the study of protein folding.

**5. MOLECULAR FRAGMENT AND FUNCTIONAL GROUP STUDIES**

The quantum chemistry of molecular fragments and functional groups is placed on a new basis:

P.G. Mezey: "Functional Groups in Quantum Chemistry" *Adv. Quantum Chem.* **1996,** *27,* 163-222 [paper 259]

A systematic approach is developed for the quantum chemical study of functional groups.

P.G. Mezey, Fuzzy Electron Density Fragments in Macromolecular Quantum Chemistry, Combinatorial Quantum Chemistry, Functional Group Analysis, and Shape – Activity Relations, Accounts of Chem. Research, **47**, 2821-2827 (2014) , invited paper.

**EVIDENCE OF IMPACT:**

1. During the past one and a half decade, the Holographic Electron Density Theorem of Prof. Mezey has been employed by several independent research groups internationally, in Germany, Spain, Belgium, Japan, China, Russia, USA, Canada, as evidenced by their numerous publications.

2. A review of Prof. Mezey's book, "Shape in Chemistry: An Introduction to Molecular Shape and Topology" (VCH: New York, 1993) writes "Mezey is the most significant contributor to the discussion on molecular shape in the latter half of the twentieth century" (Angew. Chem., Int. Ed. Eng. **1993,** 34, 361).

3. Scientific contributions of Prof. Mezey and their impact have been reviewed on three occasions by Chemistry & Engineering News (C&EN), the official publication of the American Chemical Society: C&EN, May 9, 1983, p45; C&EN, Jan.22, 1990, p18; C&EN, Aug.14, 1995, p29.

4. In the past decade, over 120 invited lectures were given at international conferences, Universities and industry.

**"Regularities in the Changes of Local and Global Chirality Measures of Natural Amino Acids in Enantiomerization Processes"**

In collaboration with Noriko Fujii, Ph.D., Professor, Radiation Biochemistry and Biological Function, Division of Radiation Life Science, Dept. of Radiation Life Science and Radiation Medical Science, Research Reactor Institute, Kyoto University
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As a continuation of earlier collaboration in the summer of 2015 (two papers are in preparation), the planned research will explore how the changes of chirality measures of the natural amino acids during enantiomerization processes correlate with the energy requirements of these processes. Some of such processes often have significant biochemical, and even health effects, such as cataract formation in the eye.

As it has been demonstrated in earlier studies [1-9], there is a variety of chirality measures, some of which can be derived from the shape calculated electron densities of molecules, but some alternative approaches rely on the coordinates of the nuclei. The interrelations among such measures and experimentally observed molecular behavior will be explored.

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