MICHEL DUPUIS
Research Professor

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Professional Research Interests and Expertise

Our research interests are in the area of theory and computation for chemistry and materials relevant to new energy technologies, in particular using multi-scale and multi-physics models and large scale computations. Our goals are to gain fu/ndamental understanding of chemistry and materials that leads to predictive design. Current research includes energy conversion materials (catalysis, photocatalysis, photovoltaics) and energy storage materials (fuel cells, batteries). Our expertise includes: electronic structure of molecules and materials, spectroscopy of molecules and solids, chemical reaction pathways, rates, and mechanisms, electron transfer processes, and transport of molecules and charge carriers in complex chemical environments. My interests and expertise include also the development of quantum chemical methods and algorithms for molecules and solids.

In 2005 I was elected a Member of the International Academy of Quantum Molecular Science, a Fellow of the American Physical Society in 2007, and a Fellow of the American Association for the Advancement of Sciences in 2008 for contributions to the advancement of the quantum molecular sciences, including the development of electronic structure software suites (HONDO, GAMESS, and NWCHEM). I am author and co-author of ~ 227 publications with ~ 28000 citations with an H-index ~ 52, and ~ 167 invited talks.

Professional Experience

- 2015-present Research Professor, Department of Chemical and Biological Engineering, University at Buffalo SUNY
- 2015-present Core member, Computation and Data-Enabled Science and Engineering Program University at Buffalo, SUNY
- 2015-2019 Assistant Director, Institute for Research and Education in Energy, Environment, and Water (RENEW), University at Buffalo, SUNY
- 2015-2019 "1000 Talents" Senior Scholar Professor, Dalian Institute of Chemical Physics, Dalian, China
- 1995-2014 Laboratory Fellow, Pacific Northwest National Laboratory, Richland, WA
- 2006-2014 Associate Division Director, Catalysis Science, Physical Sciences Division, Pacific Northwest National Laboratory, Richland, WA
- 2006-2014 Adjunct Professor, Department of Computer Sciences and Electrical Engineering, Washington State University Tri-cities, Richland, WA
- 1984-1995 Senior Scientist, IBM Corporation, Scientific and Engineering Applications Department, Kingston, NY
- 1978-1984 Staff Scientist, Lawrence Berkeley National Laboratory, National Resource for Computations in Chemistry, Berkeley, CA
- 1976-1978 Postdoctoral Scientist, IBM Corporation, San Jose, CA
- 1976 Ph.D. in Theoretical Chemistry, University at Buffalo, SUNY, Buffalo, NY Advisor: Professor Harry F. King
- 1971 Diplome d'Ingenieur, Ecole Polytechnique, Paris, France

Professional Affiliation

- International Academy of Quantum Molecular Science
- American Chemical Society
- American Physical Society
- American Association for the Advancement of Science

Honors and Distinctions

- Elected a Fellow of the American Association for the Advancement of Science (2008).
- Elected a Fellow of the American Physical Society (2007).
- Elected a Member of the International Academy of Quantum Molecular Science (2005).
- *1000 Talents Senior Scholar*, Chinese Academy of Sciences, Dalian Institute of Chemical Physics, Dalian, China (2015-2019)
- Chair, 4th Conference on "Theory and Applications of Computational Chemistry", Seattle, WA (September **2016**); including ~ 370 participants, ~ 150 talks, ~ 225 posters.
- DOE Peer Review panel for the Joint Center for Artificial Photosynthesis (JCAP) (May 2017)
- DOE Peer Review panel for DOE/BES Nanoscience Research Center (June 2013)
- Breakout session leader, Council for Chemical Research workshop on "Harnessing the Department of Energy's High-Performance Computing Expertise to Strengthen the U.S. Chemical Enterprise" (March 2011)
- Appointed to the Advisory Board for the Journal of Physical Chemistry (2009-2011).
- Adjunct Professor, Department of Computer Sciences and Electrical Engineering, Washington State University Tri-cities (2006-present).
- Adjunct Fellow, Center for Quantum Life Sciences, University of Hiroshima (Nov. 2003-2008)
- Specialist Editor, Computer Physics Communication (1998-2010)
- Peer-elected Member of the PNNL Laboratory Fellow's Executive Committee, (2002-2005; 2008-2010, 2013-present)
- Guest Professor, University of Hiroshima (Nov. 2001, Nov. 2002)
- Guest Professor, University of Tokyo (Oct-Nov. 2000)
- Fellow of Japan Society for the Promotion of Science (JSPS), University of Tokyo (Jan-Feb. 1998)
- DoD Peer Review Panel in Common High Performance Computing Support initiative, Computational Chemistry And Material Science (Sep.1996, Nov.1998)
- Guest Professor, University of Tokyo (Feb.1996)
- DOE Peer Review Panel in Computational Biochemistry (1994)
- AFOSR Chemical Sciences Review Panel (1992-1995)
- R&D 100 from R&D Magazine, "Molecular Sciences Software Suite (MS^3)", J.A. Nichols, D.R. Jones, R.J. Harrison, R.A. Kendall, T.P. Straatsma, M. Dupuis, K.P. Wolinski, E. Apra, J. Nieplocha, G.I.F ann, Rik,J. Littlefield, T.L. Keller, K.L. Schuchardt, D.K. Gracio, G. Black, and G. Thomas, 1999.
- Publication #2 (*J. Chem. Phys.* ***1976***, 65, 111) included in "*An incomplete list of landmark papers in ab initio molecular electronic structure methods*", in "Quantum Chemistry" by H.F. Schaefer III, Oxford Science Publications, 1984.

Teaching and Mentoring:

- Mathematics and Computation for Chemical Engineers – Fall semester, 2015-present
- High-Performance Computing II – Spring semester, 2016- present
- Mentoring – 2015-present: 2 PhD students, 5 MS Student, 2 Under-Graduate Students

External collaborators (last 4 years)

Deskins, Nathaniel A. Worcester Polytechnic Institute, MA

Liu, Taifeng	Henan University, Kaifeng, China
Li, Can	Dalian Institute of Chemical Physics, Dalian, China

Advisors

Ph.D. dissertation:	Harry F. King, State University of New York at Buffalo, NY
Postdoc mentor:	Bowen Liu, IBM Research Laboratory, Almaden, CA
Professional mentors:	William A. Lester Jr., Lawrence Berkeley National Laboratory, CA
	Enrico Clementi, IBM, Kingston, NY

Thesis advisor

Ms. Ginovska, Bojana (MS), Pacific Northwest National Laboratory; Ms. Nallapu, Meghana (MS), University at Buffalo; Ms. Mei, Yuhan (MS), Worcester Polytechnic Institute ; Mr. Wang, Xiaoyu (MS), University at Buffalo; Ms. Li, Dan, Univesity at Buffalo.

Postdoctoral mentor

Douali, Latifa (Teacher, Morroco); Furuhama, Ayako (Riken, Japan); Venkatnathan, Arun (Professor, IISER, Pune, India); Idipulapati, Nagesh (deceased); Iordanova, Nellie (Professor, Western Georgia University, GA, USA); Smith, Dayle (Staff, Intel Corp., USA); Deskins, Aaron (Professor, Worcester Polytechnic Institute, MA, USA); Tyminska, Nina (Postdoc, University of Wisconsin-Madison, WI)

Projects

1. "Charge Carrier Space-Charge Dynamics in Complex Materials for Solar Energy Conversion: Multiscale Computation and Simulation", **PI**, DOE Office of Basic Energy Sciences, $320K, 2018-2020
2. "Atomic-Metal-rich Carbon Electrocatalysts for Sustainable Energy via CO2 Reduction", **co-P**I, Prof. L. Velarde (UB) PI, RENEW Institute, University at Buffalo, $35K, 2017-18
3. "Toward Rational Design of Next-Generation Renewable Energy Materials: Photovoltaics from Materials to Device Model ", **co-PI**, Prof. A. Akimov (UB) PI, RENEW Institute, University at Buffalo, $35K, 2016-17
4. Energy Frontier Research Center (EFRC) "Molecular Electrocatalyis", **co-PI and Theory Task Lead**, R. M. Bullock, PI, DOE Office of Basic Energy Sciences, $4.5M/year, FY09 to FY14.
5. "Charge Transfer, Transport, and Reactivity in Complex Molecular Environments: Theoretical Studies for the Hydrogen Fuel Initiative", **PI**, DOE Office of Basic Energy Sciences, $1.15M/year, FY04 to FY10.
6. "Reaction Specificity of Nanoparticle in Solution", **co-investigator** with D. Baer (PI) and P.Tratnyek (co-PI), DOE Office of Basic Energy Sciences and Office of Environmental Management, $800K/year, FY02 to FY11.
7. "Controlling the Thermal and Non-Thermal Reactivities of Metal Oxide Structures Through Nanoscaling", **co-PI**, M. Henderson (PI), DOE Office of Basic Energy Sciences, $900K/year, FY03 to FY09.
8. "Mechanisms and Kinetics of Organic Aging and Characterization of Intermediates in High-Level wastes", **co-PI** with D. M. Camaioni (PI), FY2001 Environmental Management Science Program, DOE Office of Science and Office of Environmental Management. $810K for FY02 through FY04, FY05 to FY07.
9. "Computational Tools for Proton Transport in Complex Materials", **co-PI**, G.K.Schenter (PI), LDRD, $100K/year FY05 to FY07.
10. "Molecular Energetics of Clustered Damaged Sites", **PI**, DOE Office of Biological and Environmental Remediation, $240K/year FY02 to FY05.
11. "Molecular Modeling of Complex Reactions: The respiratory Enzyme Flavocytochrome c_3 Fumarate Reductase of *Shewanella frigidimarina*", **co-PI** with T.P. Straatsma (PI) and E.R. Vorpagel, DOE Office of Science, Advanced Modeling and Simulation of Biological Systems, $305K/year for FY02 to FY04.
12. "Quantum Calculations with 10^4-10^5 Atoms: Application to Nano-Materials and Biochemical Reactivity", **co-PI** with M. Gutowski, LDRD, Computer Science & Engineering Initiative, $170K in FY02.
13. "Mixed Hamiltonian (PW/MM) Methods for Electronic Structure Studies", **co-PI** with E.J. Bylaska and J.R. Rustad, LDRD, Computer Science & Engineering Initiative, $133K in FY00, $100K in FY01, $80K in FY02

14. "Computational Studies of Oxidant Reactions of VOC's Relevant to Tropospheric Ozone Formation", **PI**, EMSL, PNNL; Laboratory-directed Research And Development (LDRD) $97K in FY00, $100K in FY01, and $100K in FY02
15. "Computational Investigation of Acid-Base, Surface Complexation, and Oxidation/Reduction reaction mechanisms on Iron oxide and Iron Silicate Surfaces", **co-investigator** with JR Rustad (PI) and AR Felmy, DA Dixon, DOE-BES-Geosciences.
16. "Charge Transfer, Transport, and Reactivity in Complex Molecular Environments: Theoretical Studies for the Hydrogen Fuel Initiative", **PI**, DOE office of Basic Energy Sciences, $350K/year, FY05 to FY11.
17. "Biochemistry EMSL Grand Challenge: Theory and Simulations", **co-PI** with K. Rosso (PI), LDRD, $200K/year FY05 through FY06.
18. "Computational Thermochemistry: a High Performance Computing Application For The Chemical Industry", 11/1996 to 11/1997, **co-PI** with R.Harrison, D.R.Jones, D.A.Dixon, and T.H.Dunning,Jr. , EMSL, PNNL.
19. "Theoretical Studies of Formyl Radical Formation in Selected Combustion Reactions", NASA Contract No. A86130B, 10/1981 to 10/1983, **co-PI** with W.A.Lester,Jr, $ 150K.

Representative Recent Publications *(Total number of publications = 227, H-index = 52, citations ~ 28000; over 14000 citations for paper # 82; ~ 167 invited lectures)*

1. T. Liu, V. Pasumarthi, C. LaPorte, Z. Feng, Q. Li, J. Yang, C. Li, and **M. Dupuis**, "Bimodal hole transport in bulk $BiVO_4$ from computation", J. Mater. Chem. A 6, 3714 (2018).
2. S. Kerisit, K.M. Rosso, **M. Dupuis**, and M. Valiev, "Molecular Computational Investigation of Electron Transfer Kinetics Across Cytochrome-Iron oxide Interfaces", J. Phys. Chem. C 111, 11363 (2007).
3. N. A. Deskins and **M. Dupuis**, "Electron Transport via Polaron Hopping in Bulk TiO2: a Density Functional Theory Characterization", Phys. Rev. B 75, 195212 (2007).
4. N. A. Deskins, R. Rousseau, and **M. Dupuis**, "Defining the role of excess electrons in the surface chemistry of TiO_2", J. Phys. Chem. Letters, 114, 5891 (2010).
5. N. Tyminska, G. Wu, and **M. Dupuis**, "Reduced BaTiO3 as Oxygen Evolution Reaction Catalyst: a Computational Study", J. of Physical Chemistry C 121, 8378 (2017).
6. Z. Chen, Z. Duan, Z. Wang, X. Liu, L. Gu, F. Zhang, **M. Dupuis**, and C. Li, "Amorphous Cobalt Oxide Nano-particles as Active Water Oxidation Catalysts", ChemCatChem 9, 3641 (2017).
7. R. Devanathan and **M. Dupuis**, "Insight from Molecular Modeling: does the polymer side chain length matter for transport properties of perfluorosulfonic acid membranes?" Phys. Chem. Chem. Phys. 14, 11281 (2012). (cover)
8. S. Raugei, D. L. DuBois, R. Rousseau, S. Chen, M. H. Ho, R. M. Bullock, and **M. Dupuis**, "Toward Molecular Catalyst by Computer", Accts. Chem. Res. 48, 248 (2015).
9. J. Guan, Z. Duan, F. Zhang, S. D. Kelly, R. Si, **M. Dupuis**, Q. Huang, J. Q. Chen, C. Tang, and C. Li, "Water oxidation on a mononuclear manganese heterogeneous catalyst", Nature Catalysis, 1, 870 (2018).
10. N.A. Deskins, P.M. Rao, and **M. Dupuis**, "Charge Carrier Management in Semiconductors: Modeling Charge Transport and Recombination", Springer Handbook of Inorganic Photochemistry, 2019.

Publications

1. H. F. King and **M. Dupuis**, "Numerical Integration Using Rys Polynomials", J.Comp.Phys. 21, 144 (1976).
2. **M. Dupuis**, J. Rys, and H.F. King, "Evaluation of Molecular Integrals Over Gaussian Basis Functions", J.Chem.Phys. 65, 111 (1976).
3. **M. Dupuis** and H.F. King, "Molecular Symmetry And Closed-Shell SCF Calculations I", Inter.J.Quant.Chem. 11, 613 (1977).
4. **M. Dupuis** and H.F. King, "Molecular Symmetry II: Gradient of Electronic Energy With Respect to Nuclear Coordinates", J.Chem.Phys. 68, 3998 (1978).
5. **M. Dupuis** and B. Liu, "The Electronic Structure of B_2", J.Chem.Phys. 68, 2902 (1978).
6. J. Pacansky and **M. Dupuis**, "The Structure of The Ethyl Radical", J.Chem.Phys. 68, 4276 (1978).
7. J. Pacansky and **M. Dupuis**, "Ab Initio Study of The Structure of Propane and n-propyl Radical", J.Chem.Phys. 71, 2095 (1979).
8. J. Pacansky and **M. Dupuis**, "Ab Initio Study of the Isopropyl Radical", J.Chem.Phys. 73, 1867 (1980).
9. R. Schinke, **M. Dupuis,** and W.A. Lester,Jr., "Proton-H_2 Scattering on an Ab Initio CI Potential Energy Surface I: Vibrational Excitation at 10 eV", J.Chem.Phys. 72, 3909 (1980).

10. **M. Dupuis** and B. Liu, "Theoretical Study of C_2 and C_2^-, J.Chem.Phys. 73, 337 (1980).
11. D. Spangler, J.J. Wendoloski, **M. Dupuis**, M.M.L. Chen, and H.F. Schaefer III, "Geometry And Electronic Structure of $(CO)_3NiCH_2$: A Model Transition Metal Carbene", J.Am.Chem.Soc. 103, 3985 (1981).
12. **M. Dupuis**, "Energy Derivatives For CI Wavefunctions", J.Chem.Phys. 74, 5758 (1981).
13. T. Takada, **M. Dupuis**, and H.F. King, "Molecular Symmetry III: Second Derivatives of The Energy With Respect to Nuclear Coordinates", J.Chem.Phys.75, 332 (1981).
14. Y. Osamura, H.F. Schaefer III, **M. Dupuis**, and W.A. Lester,Jr., "A Unimolecular Reaction ABC = A + B + C Involving Three Product Molecules And A Single Transition State. Photodissociation of Glyoxal: HCOHCO = H_2 + CO + CO", J.Chem.Phys. 75, 5828 (1981).
15. **M. Dupuis**, J.J. Wendoloski, T. Takada, and W.A. Lester,Jr., "Theoretical Study of electrophilic Addition: $O(^3P)$ + C_2H_4", J.Chem.Phys. 76, 481 (1982).
16. **M. Dupuis**, J.J. Wendoloski, and W.A. Lester,Jr., "Electronic Structure of Vinoxy Radical CH_2CHO", J.Chem.Phys. 76, 488 (1982).
17. T. Takada and **M. Dupuis**, "On The Electronic Structure of Cubene C_8H_6", Chem.Phys.Letts. 93, 193 (1982).
18. **M. Dupuis** and J. Pacansky, "Theoretical Study of Cyclopropane And Cyclopropyl Radical: Structure And Vibrational Analysis", J.Chem.Phys. 76, 2511 (1982).
19. J. Pacansky and **M. Dupuis**, "Assignement of The Infrared Spectrum of The Ethyl Radical", J.Am.Chem.Soc. 104, 415 (1982).
20. T. Takada, **M. Dupuis**, and H.F. King, "Molecular Symmetry IV: The Coupled Perturbed Hartree-Fock Method", J.Comp.Chem. 4, 234 (1983).
21. T. Takada and **M. Dupuis**, "Theoretical Study of The Allyl Radical: Structure And Vibrational Analysis", J.Am.Chem.Soc. 105, 1713 (1983).
22. N. Abusalbi, R.A. Eades, T. Nam, D. Thirumalai, D.A. Dixon, D.G. Thrular, and **M. Dupuis**, "Electron Scattering by Methane: Elastic Scattering and Rotational Excitation Cross-sections Calculated With Ab Initio Interaction Potentials", J.Chem.Phys. 78, 1213 (1983).
23. J. Rys, **M. Dupuis**, and H.F. King, "Computation of Electron Repulsion Integrals Using The Rys Quadrature Method", J.Comp.Chem. 4, 154 (1983).
24. S. Chapman, **M. Dupuis**, and S.Green, "Theoretical Three-Dimensional Potential Energy Surface For The Reaction of Be with HF", Chem.Phys. 78, 93 (1983).
25. M.E. Colvin, G.P. Raine, H.F. Schaefer,III, and **M. Dupuis**, "Infrared Intensities of H_3O^+, H_2DO^+, HD_2O^+, and D_3O^+", J.Chem.Phys. 79,1551 (1983).
26. **M. Dupuis**, W.A. Lester,Jr., B.H. Lengsfield and B. Liu, "Accurate MCHF/CI Calculation of the H_2CO = H_2 + CO Dissociation", J.Chem.Phys. 79, 6167 (1983).
27. **M. Dupuis** and W.A. Lester,Jr., "Hydrogen Atom Migration in The Oxidation of Aldehydes: $O(^3P)$ + H_2CO", J.Chem.Phys. 80, 4193 (1984).
28. **M. Dupuis** and W.A. Lester,Jr., "Hydrogen Atom Abstraction From Aldehydes: OH + H_2CO And O + H_2CO", J.Chem.Phys. 81, 847 (1984).
29. **M. Dupuis** and J.J. Wendoloski, "Systematic GVB Study of Harmonic Vibrational Frequencies And Dipole Moment Derivatives: The Vinyl Radical C_2H_3 And Other simple Molecules", J.Chem.Phys. 80, 5698 (1984).
30. V.Z. Kresin, W.A. Lester,Jr., **M. Dupuis**, and C.E. Dateo, "Chemical Reaction as a Quantum Transition", Intern.J.Quant.Chem. S18, 691 (1984).
31. R.M. Grimes, **M. Dupuis**, and W.A. Lester,Jr. "Static Dipole Polarizability of Electronically Excited Molecules: $H_2(B^1\Sigma_u^+)$", Chem.Phys.Lett. 110, 247 (1984).
32. C.E. Dateo, **M. Dupuis**, and W.A. Lester,Jr., "Ab Initio Study of Cyanogen C_2N_2: The $X^1\Sigma_g^+$, $a^3\Sigma_u^+$, $B^1\Delta_u$ and $C^1\Pi_u$ States", J.Chem.Phys. 83, 265 (1985).
33. M.W. Schmidt, M.S. Gordon, and **M. Dupuis**, "The Intrinsic Reaction Coordinate And The Rotational Barrier in Silaethylene", J.Am.Chem.Soc. 107, 2585 (1985).
34. **M. Dupuis** and W.A. Lester,Jr., "Low-lying Electronic States of Nitrosyl Cyanide NCNO: an Ab Initio MCHF Study", J.Chem.Phys. 83, 3990 (1985).
35. **M. Dupuis**, G. Fitzerald, B. Hammond, W.A. Lester,Jr., and H.F.Schaefer,III, "Theoretical Study of the H + O_3 = OH + O_2 = O + HO_2 System", J.Chem.Phys. 84, 2691 (1986).
36. K.S. Kim, **M. Dupuis**, G.C. Lie, and E. Clementi, "Revisiting Small Clusters of Water Molecules", Chem.Phys.Lett. 131, 451 (1986).
37. **M. Dupuis** and J.D. Watts, "Parallel Computation of Molecular Energy Gradients on The Loosely Coupled Array of Processors (LCAP)", Theor.Chim.Acta 71, 91 (1987).
38. **M. Dupuis** and W.A. Lester, "One-Electron Property From MCHF Wavefunction: The Dipole Moment of Ozone", Theor.Chim.Acta 71, 255 (1987).

39. C.E. Dateo, V.Z. Kresin, **M. Dupuis**, and W.A.Lester,Jr., "Photodissociation as a Quantum Transition: Photofragment Vibrational Distributions of C_2N_2 ($1\Pi_u$) Predissociation", J.Chem.Phys. 86, 2639 (1987).
40. P. Otto and **M. Dupuis**, "Ab initio Hartre-Fock Energy Band Structure Calculations on Polyaniline", J.Chem.Phys. 86, 6309 (1987).
41. *F. Sim, C.R.A. Catlow, **M. Dupuis**, J.D. Watts, and E. Clementi, "Ab initio SCF-MO Calculations on Inorganic Materials with the Inclusion of long-range Coulomb Effects: α-Quartz and Defects", in "Supercomputer Research in Chemistry and Chemical Engineering", ACS Symposium Series 353, D.G.Truhlar and K.Jensen Eds., 1987.*
42. ***M. Dupuis**, H.O. Villar, and E. Clementi, "Quantum Mechanical Simulations of Polymers for Molecular Electronics and Photonics", in "Supercomputer Research in Chemistry and Chemical Engineering", ACS Symposium Series 353, D.G.Truhlar and K.Jensen Eds., 1987.*
43. H.O. Villar and **M. Dupuis**, "Bond Orders And Valencies From Ab Initio Wavefunctions: Application to Prototypical Molecules And to the Characterization of Solitons in Polyenes.", Chem. Phys. Lett. 142, 59 (1987).
44. H.O. Villar, **M. Dupuis**, J.D. Watts, G.J.B. Hurst, and E. Clementi, "Structure, Vibrational Spectra, and Infrared Intensities of Polyenes From Ab Initio SCF Calculations", J.Chem.Phys. 88, 1003 (1988).
45. H.O. Villar and **M. Dupuis**, "Ab Initio Study of Charged Polyenes as Charge Carrier Models in Conducting Polymers", Phys. Rev. B . 37, 2520 (1988).
46. H.O. Villar, **M. Dupuis**, and E. Clementi, "Defects in Doped Polyacetylene : Ab Initio Infrared And Raman Spectroscopy of Solitons", J.Chem.Phys. 88, 2859 (1988).
47. G.J.B. Hurst and **M. Dupuis**, "Integral Data Compression for the FPS 64 bit Processors: Improved I/O and Reduced Storage", J.Comp.Chem. 9, 148 (1988).
48. J.D. Watts and **M. Dupuis**, "Parallel Computation of the Moller-PlessetSecond-Order Contribution to the Electronic Correlation Energy",J.Comp.Chem. 9, 158 (1988).
49. G.J.B. Hurst, **M. Dupuis**, and E. Clementi, "Ab Initio Analytic Polarizability, First and Second Hyperpolarizabilities of Large Conjugated Organic Molecules: Applications to Polyenes C_4H_6 to $C_{22}H_{24}$", J.Chem.Phys. 89, 385 (1988).
50. **M. Dupuis**, J.D. Watts, H.O. Villar, and G.J.B. Hurst, "The General Atomic And Molecular Electronic Structure System HONDO 7.0", Computer Physics Communications, 52, 415 (1989).
51. E. Clementi, S. Chin, G. Corongiu, J.H. Detrich, **M. Dupuis**, D. Folsom, G.C. Lie, D. Logan, and V. Sonnad, "Supercomputing and Supercomputer for Science and Engineering in General, and for Chemistry and Biosciences in Particular", Intern.J.Quant.Chem. 35, 3 (1989).
52. E. Perrin, P.N. Prasad, P. Mougenot, and **M. Dupuis**, "Ab Initio Calculations of Polarizability And Second Hyperpolarizability in Benzene Including Electron Correlation Treated by Moeller-Plesset Theory", J.Chem.Phys. 91, 4728 (1989).
53. U. Niesar, G. Corongiu, M.J. Huang, **M. Dupuis**, and E. Clementi, "Preliminary Observations on a New Water-Water Potential", Intern.J.Quant.Chem. S23, 412 (1989).
54. P. Mougenot and **M. Dupuis**, "Electronic Structure of the Hydroxy-Vinoxy Radical HO-CH-CHO", Chem.Phys.Letters, 165, 87 (1990).
55. S. Karna, **M. Dupuis**, E. Perrin, and P.N. Prasad, "Ab Initio Calculations of Polarizability And First And Second Hyperpolarizabilities of CHF_3, $CHCl_3$, $CHBr_3$, and CHI_3 Using Effective Core Potentials", J.Chem.Phys. 92, 7418 (1990).
56. A. Farazdel, **M. Dupuis**, E. Clementi, and A. Aviram, "Electric-Field Induced Intramolecular Electron Transfer in Spiro π-electron Systems, and Their Suitability as Molecular Electronic Devices. A Theoretical Study.", J.Am.Chem.Soc. 112, 4206 (1990).
57. J. Ciolowski, T. Hamilton, G. Scuseria, B.A. Hess,Jr., J. Hu, L.J. Schaad, and **M. Dupuis**, "Application of the GAPT Population Analysis to Some Organic Molecules and Transition States", J.Am.Chem.Soc. 112, 4183 (1990).
58. C. Daniel and **M. Dupuis**, "Nonlinear Optical Properties of Organic Solids: Ab Initio Polarizability and hyperpolarizabilities of Nitroaniline Derivatives ", Chem.Phys.Lett. 171, 209 (1990).
59. S. Karna and **M. Dupuis**, "Frequency Dependent Hyperpolarizabilities of Haloforms From Ab Initio SCF Calculations", Chem. Phys. Lett. 171, 201 (1990).
60. S.A. Maluendes and **M. Dupuis**, "A Dynamic Reaction Coordinate Approach to ab initio Reaction Pathways: Application to the 1,5-hexadiene Cope Rearrangement", J.Chem.Phys. 93, 5902 (1990).
61. B.L. Hammond, S.Y. Huang, W.A. Lester,Jr., and **M. Dupuis**, "Theoretical Study of the O(^{3}P) + Allene Reaction", J.Phys.Chem. 94, 7969 (1990).
62. C.X. Cui, M. Kertesz, and **M. Dupuis**, "Ab Initio Oligomer Calculations of Dynamic Properties of Polyacetylene", J.Chem.Phys. 93, 5890 (1990).

63. P.R. Seidl, J.W. De M.Carneiro, J.G.R. Tostes, C.A. Taft, and **M. Dupuis**," Ab Initio Charge Distribution in Tetracyclic Norbornyl Derivatives ", Chem.Phys.Lett. 175, 182 (1990).
64. S. Karna, P.N. Prasad, and **M. Dupuis**, "Nonlinear Optical Properties of Para-NitroAniline : an Ab Initio Time-dependent Coupled Perturbed Hartree-Fock Study", J.Chem.Phys. 94, 1171 (1991).
65. A. Farazdel and **M. Dupuis**, "On The Determination of The Minimum on the Crossing Seam of Two Potential Energy Surfaces", J.Comp.Chem. 12, 276 (1991).
66. S. Karna and **M. Dupuis**, "Time-Dependent Coupled Perturbed Hartree-Fock Theory for Frequency Dependent Nonlinear Optical Phenomena", J.Comp.Chem. 12, 487 (1991).
67. A. Farazdel and **M. Dupuis**, "All-Electron ab Initio SCF Study of Electron Transfer in Scanning Tunneling Microscopy at Large and Small Tip-sample Separations: Supermolecule Approach", Phys.Rev.B , 44 , 3909 (1991).
68. J. Perez and **M. Dupuis**, "Hydrogen Bonds And (Hyper)polarizabilities in Molecular Crystals : an Ab Initio SCF Study of Urea", J.Phys.Chem. 95, 6525 (1991).
69. S. Karna, E. Perrin, P.N. Prasad, and **M. Dupuis**, "Dynamic Polarizability of Haloforms: Experimental and Ab Initio Theoretical Studies", J.Phys.Chem. 95, 4329 (1991).
70. F. Sim, D.R. Salahub, S. Chin, and **M. Dupuis**, "LCGTO-LSD Calculations on the Allyl And Polyene Radicals: C_3H_5 to $C_{11}H_{13}$", J.Chem.Phys. 95, 4317 (1991).
71. F. Sim, C.R.A. Catlow, **M. Dupuis**, and J.D. Watts, "Hartree-Fock Calculations on Defects in &alpha.-Quartz", J.Chem.Phys. 95, 4215 (1991).
72. **M. Dupuis**, C. Murray, and E. R. Davidson, "The Cope Rearrangement Revisited", J.Am.Chem.Soc. 113, 9756 (1991).
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193. S. Chen, R. Rousseau, S. Raugei, **M. Dupuis**, D. L. DuBois, and R. M. Bullock, "Comprehensive Thermodynamics of Nickel Hydride Bis(Diphosphine) Complexes: A Predictive Model through Computations," Organometallics, 30, 6108 (2011).
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196. S. Raugei, S. Chen, R. Rousseau, S. Raugei, **M. Dupuis**, D. L. DuBois, and R. M. Bullock, "The role of pendant in the breaking and forming of molecular hydrogen catalyzed by nickel complexes," Chem. A Eur. J. 18, 6493 (2012).
197. R. Devanathan, N. Idupulapati, and **M. Dupuis**, "Molecular modeling of the morphology and transport properties of two direct methanol fuel cell membranes: Phenylated sulfonated poly(ether ether ketone ketone) versus nafion" J. Mat. Res. 27, 1927 (2012).
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202. R. Devanathan, N. Idupulapati, M. D. Baer, C. M. Mundy, and **M. Dupuis**, "Ab initio molecular dynamics simulation of proton hopping in a model polymer membrane", J. Phys. Chem. B 117, 16522 (2013).
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205. N. A. Deskins, R. Rousseau, and **M. Dupuis**, "Correction to 'Localized Electronic States from Surface Hydroxyls and Polarons in TiO_2(110)', 'Defining the Role of Excess Electrons in the Surface Chemistry of TiO_2', and 'Distribution of Ti^{3+} Surface Sites in Reduced TiO_2', J. Phys. Chem C 118, 13326 (2014).
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Other Articles and Chapters

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2. W.A. Lester,Jr., **M. Dupuis**, T.J. O'Donnell and A.J. Olson, "Some Computational Trends in Theoretical Chemistry", IUPAC Frontiers of Chemistry, K.J.Laidler Editor, Pergamon Press, 1982.
3. R.M. Grimes, **M. Dupuis** and W.A. Lester,Jr., "Theoretical Study of intermolecular Energy Transfer of an Electronically Excited Diatomic Molecule by Atom Impact: $He(^1S) + H_2 (B1\Sigma_u^+)$", 1985 National Organization of Black Chemists and Chemical Engineers.
4. **M. Dupuis** and H.F. King, "Energy Derivatives and Symmetry" in "Geometrical Derivatives of Energy Surfaces and Molecular Properties", edited by P. Jorgensen and J. Simon, NATO ASI Series C166, Reidel 1986.
5. **M. Dupuis**, H.O. Villar, G.J.B. Hurst, and E. Clementi, "Supercomputer Quantum Simulations For Electronic Devices at The Molecular Level" in Proceedings of the Third International Conference on Supercomputing, Boston, 1988.
6. E. Clementi, S. Chin, G. Corongiu, **M. Dupuis**, G.C. Lie, and V. Sonnad, "Modern Computational Chemistry", Proceedings of the Third International Conference on Supercomputing, Boston, 1988.
7. E. Clementi and S. Chin, G. Corongiu, J.H. Detrich, **M. Dupuis**, D. Folsom, G.C. Lie, D. Logan, V. Sonnad, "Supercomputing and Supercomputers : For Science and Engineering in General, and for Chemistry and Biosciences in Particular", in "Biological And Artificial Intelligence Systems", E.Clementi and S. Chin Editors, Escom Science Publishers (1988).
8. **M. Dupuis**, and E. Clementi, "Electronic Devices from Molecules: Overview, Prospects, and Theoretical Chemistry", in "Biological And Artificial Intelligence Systems", E.Clementi and S. Chin Editors, Escom Science Publishers (1988).
9. **M. Dupuis**, "The HONDO Program : Overview And Algorithms, Including Integral and Symmetry Techniques, Using Vector and Parallel Processing ", in Proceedings of workshop on "Quantum Chemistry : Basics and Trends ", R.A. Carbo Editor, Studies in Physical and Theoretical Chemistry, Vol. 62, p.59, Elvesier Science Publishers B.V., Amsterdam (1989).
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11. **M. Dupuis**, P. Mougenot, R. Lindh, K. Dyall, and B. Liu, "HONDO8: a General Atomic And Molecular Electronic Structure System", Proceedings of the Fourth International Conference on Supercomputing, Santa Clara, 1989.
12. **M. Dupuis**, P. Mougenot, J.D. Watts, G.J.B. Hurst, and H.O. Villar, "HONDO: A General Atomic and Molecular Electronic Structure System", in "Modern Techniques in Computational Chemistry", MOTECC-89, E. Clementi Editor, ESCOM, Leiden, 1989.
13. **M. Dupuis**, A. Farazdel, S.P. Karna, and S.A. Maluendes, "HONDO: A General Atomic and Molecular Electronic Structure System", in "Modern Techniques in Computational Chemistry", MOTECC-90, E. Clementi Editor, ESCOM, Leiden, 1990.
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15. E. Clementi, S. Chin, G. Corongiu, J. Detrich, **M. Dupuis**, M.J. Evans, D. Folsom, D. Frye, G.C. Lie, D. Logan, D. Meck, and V. Sonnad, "LCAP: Loosely Coupled Array of Processors Parallel Processing Systems", MOTECC-91, E. Clementi Editor, ESCOM, Leiden, 1991.
16. **M. Dupuis** and A. Marquez, "Molecular Orbital Studies of Electric Field-Controlled Electron Transfer", in Molecular Electronics Science and Technology II. A.Aviram Ed., American Institute of Physics, #262, New York, 1992.
17. **M. Dupuis**, S. Chin, and M. Marquez, "CHEM-Station and HONDO: Modern Tools for Electronic Structure Studies Including Electron Correlation", in NATO ASI series, "Electron Correlation and Relativistic Effects in Molecules and Clusters", M. Malli, Editor, Plenum Press, New York, 1993.
18. R.A. Kendall, E. Apra, D.E. Bernholdt, E.J. Bylaska, **M. Dupuis**, G.I. Fann, R.J. Harrison, J. Ju, J.A. Nichols, J. Nieplocha, T.P. Straatsma, T.L. Windus and A.T. Wong. 1996. **"High Performance Computing in Chemistry: NWChem"**. *Future Generations Computer Systems*. 128 (1 - 2):260 - 283.

19. A.M. Marquez, J. Oviedo, J. Fernandez-Sanz, and **M. Dupuis**, "Distributed Computing in Quantum Chemistry: Parallel Computation of the second derivatives of the RHF energy on distributed memory computers", EuroPVM'95, J. Dongarra et al. Editors, Hermes, Paris, 1995, p.191.
20. **M. Dupuis** and A. Marquez, "Weak Overlap and Spin Recoupling: Applications of the CAS SCF Method ", in "Advances in Multi-Reference Methods", World Scientific Press, K. Hirao Editor, 1999.
21. M.Aida, M. Kaneko, and **M. Dupuis**, "Radiation-Induced DNA Damage and Repair: An Approach from Ab Initio MO Method", in "Computational Molecular Biology", J.Leszczynski Editor, Elsevier Science B.V., 1999.
22. D.A. Dixon, T.H. Dunning,Jr., **M. Dupuis**, D. Feller, D. Gracio, R.J. Harrison, D.R. Jones, R.A. Kendall, J.A. Nichols, K. Schuchardt, and T.P. Straatsma, "Computational Chemistry in the Environmental Molecular Sciences Laboratory", in "High Performance Computing", R.J.Allan et al. Editors, Kluwer Academic / Plenum Publishers, New York, 1999.
23. M. Aida, H. Yamataka, and **M. Dupuis**, "Modeling of Reactivities of Organic Molecules by Means of ab Initio MD method" in "Large-Scale Scientific Computations of Engineering And Environmental Problems II", M.Griebel, S.Margenov, and P.Yalamov Editors, Vieweg & Sohn, Wiesbaden, p. 319, 2000.
24. T.L. Windus, E.J. Bylaska, **M. Dupuis**, S. Hirata, L. Pollack, D.M. Smith, T.P. Straatsma, E. Aprà, "NWChem: New Functionality", in Proceedings of Computational Science - ICCS 2003, International Conference, Eds. P.M.A. Sloot, D. Abramson, A. Bogdanov, J.J Dongarra, A. Zomaya, and Y. Gorbachev, vol. 2660 Lecture Notes in Computer Science (Springer-Verlag, Berlin, 2003)

Computer Programs

1. **M. Dupuis**, J. Rys, and H.F. King, 'HONDO76', Quantum Chemistry Program Exchange, (1976).
2. **M. Dupuis**, J. Rys, and H.F. King, 'HONDO-5', Quantum Chemistry Program Exchange, (1979).
3. **M. Dupuis**, J.D. Watts, H.O. Villar, and G.J.B. Hurst, 'HONDO-7', Quantum Chemistry Program Exchange, # 544 (1988); also Computer Physics Communication Program Library (1988).
4. **M. Dupuis**, 'HONDO-8' from 'MOTECC-89', IBM Corporation. Over 200 copies of HONDO7 and HONDO8 in use worldwide.
5. **M. Dupuis**, A. Marquez, And S. Chin, 'HONDO-8 From CHEM-Station', IBM Corporation,

Technical Reports

1. P.Th.VanDuijnen and **M.Dupuis**, "On the Quantum Mechanical Treatment of Solvent Effects II: Comparison of Exact And Expanded Field Operator", IBM Technical Report KGN-38, 1985.
2. Bowen-Jenkins and **M. Dupuis**, "Parallel Computation of Molecular Electronic Similarity", IBM Technical Report KGN-46 , 1985.
3. **M. Dupuis** and J.D. Watts, "Improved Hartree-Fock Calculations by Taking Advantage of The Pipeline Architecture of The FPS-X64 Processors", IBM Technical Report KGN-69, 1986.
4. **M. Dupuis**, "Performance Evaluation of the I/O FPS-D64 Subsystem: do we really need specialized Software", IBM Technical Report KGN-70, 1986.
5. J.D.Watts, **M. Dupuis**, and H.O. Villar, "Implementation of Large Fortran Programs on the Loosely Coupled Array of Processors: Parallel Computation of Molecular Energy Gradients", IBM Technical Report KGN-78, 1986.
6. J.D. Watts and **M. Dupuis**, "Towards Efficient Parallel Computation of Correlated Wavefunctions: Implementation of Integral Transformation Algorithms on LCAP", IBM Technical Report KGN-101, 1986.
7. J.D. Watts and **M. Dupuis**, "Vector and Parallel Implementation of a Fourth-order Moller-Plesset Perturbation Theory (MP4) program", IBM Technical Report KGN-197, 1986.
8. P. Mougenot and **M. Dupuis**, " The MCSCF Program in HONDO: a new code for Vectorization and Parallelization " IBM Technical Report KGN-158, 1986.

Books and Reports

1. Proceedings of NRCC Workshop on "Recent Development and Applications of Multiconfiguration Hartree-Fock Method", **M. Dupuis** Editor, 1981.
2. "Supercomputer Simulations in Chemistry", **M. Dupuis** Editor, Lecture Notes in Chemistry, Springer-Verlag, 1986.

Invited Talks and Visits

1. "Electronic Structure Aspects of Photodissociation: Application to $H_2CO = H_2 + CO$ ", Workshop on H_2CO Photodissociation, Berkeley, (Oct. 1981); IBM Research Laboratory, San Jose, (Nov. 1981); ACS National Meeting, Las Vegas, (Mar. 1982).
2. "MCHF Calculations on Midi- and Super-Computers", Sanibel Symposium on Computers in Chemistry, (Mar. 1983).
3. "Applications of the MCHF Method: Determination of the Electronic Structure of Excited States and Reaction Pathways", Physical Chemistry Seminar, University of California, Berkeley, (Apr. 1983); National Bureau of Standards, Gaithersburg, (Jun. 1983).
4. "Spectroscopy of Electronically Excited Radicals: Ab Initio Study", Atomic And Molecular Spectroscopy Seminar, University of California, Berkeley, (Feb. 1984).
5. Visiting Scientist, National Bureau of Standards, Gaithersburg, (Mar.-Apr. 1984).
6. "Ab Initio Studies of Radical Reactions", Physical Chemistry Seminar, University of Colorado, Boulder, (Sep. 1984)).
7. "Parallelism in Computational Chemistry: Applications in Quantum and Statistical Mechanics", Institute For Computer Research, University of Waterloo, (Oct. 1984); Oakridge National Laboratory, (Dec. 1984).
8. "Energy Derivatives and Molecular Symmetry", NATO Advanced Research Workshop, Sonderborg, Denmark, (Aug. 1985).
9. "The Loosely Coupled Array of Processors as a Supercomputer for Scientific Applications", Ecole Polytechnique, Montreal, (Nov. 1985).
10. "Quantum Chemistry on the Loosely Coupled Array of Processors", Workshop on "Parallel Processors in Quantum Chemistry", Edmonton, (Jul. 1986).
11. "Theoretical Chemistry on a Parallel Supercomputer", Congres des Chimistes Theoriciens d'Expression Latine, Lyon, (Jul. 1986).
12. "Water in Biological Systems", Sanibel Symposium on Quantum Biology and Quantum Pharmacology, (Mar. 1987).
13. Session Chairman, Winter Symposium on Supercomputer Research in Chemistry and Chemical Engineering, University of Minnesota, (Mar. 1987).
14. "Scientific And Engineering Applications for Supercomputers", Spring Science Seminar, Florida A&M University, (Mar. 1987).
15. "Parallel Supercomputers and Global Simulations", workshop on "Advanced Computation and Simulation of Complex Materials Phenomena", convened by the National Materials Advisory Board of the National Research Council, La Jolla (CA), (Mar. 1987).
16. Invited Lecturer, Summer School on Supercomputers, Prague, (Aug.1987; declined, no funding).
17. Invited Speaker, World Congress of Theoretical Organic Chemistry, Budapest, (Aug. 1987; declined, no funding).
18. Invited Lecturer, Ecole Normale de Paris, Paris, (May 1987; declined).
19. "Parallel Computing in Computational Chemistry", Ninth Annual West Coast Theoretical Chemistry Conference, Berkeley, (Jun. 1987).
20. "Numerically Intensive Computational Sciences", First SCCFF Meeting, Facultes Universitaires Notre-Dame de la Paix, Namur , Belgium, (Oct. 1987).
21. "Supercomputing in Computational Chemistry", Center for Computational Sciences, University of Kentucky, Lexington, (April 1988).
22. "Electronic Structure Simulations For Electronic Devices at The Molecular Level", Physical Science Seminar, IBM Almaden Research Center, San Jose, (April 1988).
23. "Quantum Supercomputer Simulations For Electronic Devices at The Molecular Level", Third International Conference on Supercomputing, Boston, (May 1988).
24. "Quantum Molecular Studies of Molecular Electronics", Workshop on Quantum Chemistry, Basic Aspects, Actual Trends, Girona, Spain, (June 1988).
25. "Electronic Devices From Molecules: Overview, Prospects, and Theoretical Chemistry", Fourth International Symposium on Biological and Artificial Intelligence Systems, Trento, Italy, (September 1988).
26. "Electronic Devices From Molecules: Structure and Dynamics from Quantum Mechanical Studies", Workshop on Chemical Reaction Dynamics, Universityof California, Berkeley, (November 1988).
27. "Quantum Mechanical Studies For Molecular Electronics", International Conference on "Molecular Electronics: Science and Technology", Hawaii, (February 1989).

28. "HONDO8: Recent Developments and Applications to Molecular Electronics", Fourth International Conference on Supercomputing, Santa Clara, (May 1989).
29. "Quantum Chemistry For Molecular Electronics", Second SCCFF Meeting, Facultes Universitaires Notre-Dame de la Paix, Namur, Belgium, (May 1989).
30. "Parallel Processing on the IBM 3090, And Extension to LCAP, With Emphasis on Chemistry", Workshop on "Parallel Computers in Chemistry", Argonne National Laboratory, Argonne, Illinois, (June 1989).
31. "Electronic Devices From Molecules: Structure and Dynamics from Quantum Mechanical Studies", Theoretical Chemistry Division, Argonne National Laboratory, (June 1989).
32. "HONDO: Overview and Applications", Symposium on Ab Initio Chemical Software, Ohio Supercomputer Institute, Columbus, Ohio, (Sep. 1989).
33. Invited Speaker, 18-th International Congress of Theoreticians of Latin Expression, La Plata, Argentina (Sept. 1989).
34. Visiting Scientist, Centro Brasiliero de Pesquisas Fisicas, Rua Dr. Xavuer Siguad, 150, 22290 Rio de Janeiro, RJ, Brazil : "Theoretical Studies of New Organic Materials: Hyperpolarizabilities and Electron Transfer for Opto-electronics", Sept. 1989.
35. "Theoretical Studies of New Organic Materials: Hyperpolarizabilities and Electron Transfer for Opto-electronics", Departamento de Quimica Fundamental, Universidade Federal de Pernambuco, 50739 Recife, PE, Brazil, Sept. 1989.
36. Session Chairman, Symposium in the Honor of Professor John Pople, H.F.Schaefer III and N.Handy Organizers, University of Georgia, Athens, Oct. 1989.
37. Invited Speaker, "Molecules in Electric Field: A Theoretical Study", Second World Congress of Theoretical Organic Chemistry, Toronto, July 1990.
38. "Recent Developments in Computational Chemistry at IBM-Kingston", Molecular Sciences Research Center, Batelle Pacific Northwest Laboratory, Richland, WA, July 1990.
39. Invited Speaker, Workshop on "Methodology of the Evaluation of Integrals in LCAO Calculations", J. Almlof Organizer, Argonne National Laboratory, Aug., 1990.
40. Invited Speaker, 1990 IBM-Europe Polymer Symposium, "Non-linear Optical Properties of Molecules From Quantum Mechanical Calculations", Oberlech, Austria, Aug. 1990
41. Invited Speaker, "Molecules in Electric Field: A Quantum MolecularStudy", 5th International Symposium on Biological and Artificial Intelligence Systems, Rome, Sep. 1990.
42. Invited Speaker, Workshop on "Ab Initio Treatment of Crystalline Systems: Hartree-Fock and Beyond", Centre Europeen de Calculs Atomiques et Moleculaires, Orsay, France, Oct. 1990.
43. Invited Speaker, APS Regional Meeting, "Supercomputing For Computational Chemistry", Poughkeepsie, Oct. 1990.
44. Invited Speaker, "Ab Initio Studies of Dynamics, Properties, and Electron Transfer of Molecules", National Institutes of Health, Bethesda, MD, Feb. 1991.
45. Invited Speaker, "Optical Properties of Molecules From Ab Initio Quantum Mechanical Calculations", Polymers and Nonlinear Optics Colloquium Series, Northwestern University, Evanston,Ill. , Feb. 1991.
46. Invited Speaker, 1st Canadian Symposium on Computational Chemistry, "Non-linear Optical Properties of Molecules from Quantum Mechanical Calculations", Oxford, Quebec, May 1991.
47. Invited Speaker, 1991 ACS Joint Central-Great Lakes Regional Meeting, "Ab Initio Non-linear Optical Properties of Molecules" IUPUI, Indianalopis, May 1991.
48. Invited Speaker, Workshop on "Calcul Scientifique et Chimie Quantique", organized by CEA, EDF, and INRIA, Roquencourt, France, May 1991.
49. Invited Speaker, "Electron Transfer in STM : A Quantum Molecular Study", Fourth SCCFF Meeting, Facultes Universitaires Notre-Dame de la Paix, Namur, Belgium, May 1991. (declined)
50. Invited Participant, "Parallel Computers in Chemical Physics", Argonne National Laboratory, July 1991.
51. Invited Speaker, Department Seminar, Wesleyan University, "Recent Advances in Theoretical Studies of Molecular Electronic Structure and Properties", Sept. 1991.
52. Invited Speaker, Physical Chemistry Seminar, University of California, Berkeley, "Recent Advances in Theoretical Studies of Molecular Electronic Structure and Properties", Oct. 1991.
53. Invited Speaker, Conference on "Current Trends in Computational Chemistry, "The CHEM-Station Graphical Environment For Modern Electronic Structure Studies in Research And Education", University of Perugia,, Italy, Oct. 1991.
54. Invited Speaker, International Conference on "Molecular Electronics: Science and Technology", "The Methods of Quantum Chemistry for Molecular Electronics", St.Thomas, Dec. 1991.
55. Invited Speaker, Sanibel Symposium on Theoretical Organic Chemistry, "The Cope Rearrangement Revisited, and Graphics-Based Studies of Chemical Reactivity", Saint Augustine, Mar. 1992.

56. Invited Speaker, NATO Workshop on "Relativistic And Electron Correlation Effect in Molecules And Solids", " Overview And Applications of HONDO, a General Atomic And Molecular Electronic Structure System ", Vancouver, Aug. 1992.
57. Invited Speaker, ACS regional meeting, symposium on Theoretical Organic Chemistry, "Recent Advances for Theoretical Organic Chemistry", Pittsburgh, Oct. 1993.
58. Invited Speaker, Nagoya Symposium on Chemical Reaction Theory, "Active Electrons and Active Orbitals In Chemical Reactions", Nagoya, Japan, Nov. 1993.
59. Invited Speaker, Pittsburgh Supercomputer Center, "Towards Massively Parallel Processing in Chemistry", Pittsburgh, Jan. 1994.
60. Invited seminar, Department of Chemistry, The Ohio State University, "Weak Overlap And Spin Recoupling in Electronic Structure", Columbus, Feb. 1994.
61. Invited Speaker, ACS National Meeting, symposium on Parallel Computing in Chemistry, "Computational Chemistry Applications for the IBM Scalable POWERParallel System", San Diego, Apr. 1994.
62. Invited Speaker, 2d Canadian Symposium on Computational Chemistry, Kingston, Ontario, May 1994.
63. Invited Speaker, IMS Workshop on Parallel Computing in Quantum Chemistry, "Chemistry Computing on the IBM SP2 Parallel Computer", Institute of Molecular Science, Okazaki, Japan, Nov. 1994.
64. Invited Speaker, Workshop on Advanced Materials for Molecular Electronics and Photonics, "HyperRaman Intensities And Other ab Initio Calculations For Nonlinear Optical Materials", Center For Research on Molecular Electronics And Photonics, University of Mons-Hainaut, Dec. 1994.
65. Invited Seminar, "Parallel Computing with HONDO : Methods and Applications", Laboratoire des Interactions Moleculaires, University Paris VII, Jussieu, Paris, Dec. 1994; Laboratoire de Chimie Quantique, Universite Louis Pasteur, Strasbourg, Dec. 1994.
66. Invited Speaker, Symposium on "Industrial Applications of Quantum Chemistry", "Modern Electronic Structure Studies in Computer-Aided Design", ACS Central Regional Meeting, Akron, Ohio, May 1995.
67. Invited Lecturer, PNL Workshop on Parallel Computational Chemistry Tutorial, NERSC-Livermore, August 7-11, 1995.
68. Invited Speaker, Symposium on "The Transition State From Dilute Gases to Condensed Media", ACS National Meeting, New Orleans, March 1996, "Method of Electronic Structure For Reaction Paths And Transition States".
69. Invited Speaker And Advisory Committee Member, Third UNAM-Cray Supercomputing Conference in Computational Chemistry, Mexico City, Aug. 1996, "Ab Initio Study of Mixed-Valence Complexes".
70. Invited Speaker, International Conference on Parallel Computing, "Advanced Techniques For High Scalability: Applications to Computational Chemistry", University of Minnesota Supercomputer Institute, Oct. 3-4, 1996 .
71. Invited Speaker, Sanibel Symposium on Theoretical Inorganic Chemistry, “Ab Initio Studies of Spin Multiplicity in Transition Metal Complexes “, Saint Augustine, Mar. 1997.
72. Invited Speaker, Symposium on "Industrial Applications of Quantum Chemistry", “Accurate Thermochemistry”, ACS Natioanl Meeting, San Fransisco, March 1997.
73. Invited Speaker, Satellite Symposium on "Structural And Mechanistic Organic Chemistry. A Tribute to Norman L. Allinger", “Accurate Thermochemistry”, University of Georgia, Athens, GA, June 1997.
74. Invited Speaker, 3d Canadian Symposium on Computational Chemistry, “Spin Multiplicities and Ab Initio Methods: a Comparative Study of Molecular Orbital Theory And Density Functional Theory”, Edmonton, Canada, July 1997.
75. Seminar Speaker, NIST, “Accurate Thermochemistry: Correlation Energy Scaling “, Gaithersburg, USA, November 1997.
76. Invited Speaker,, 6th Conference on “ Current Trends in Computational Chemistry“,“Spin Multiplicities And Ab Initio Methods: a Comparative Study of Molecular Orbital Theory And Density Functional Theory”, Jackson State University, Jackson, USA, November 1997.
77. Invited Speaker, XII International Conference on Computers in Chemical Research And Education, University of Pune, Indaia, Jan. 98. Declined
78. Invited Speaker, V Simposio de Espectroscopia Laser y Optica, Universidad del Zulia, Maracaibo, Venezuela, Oct. 99. Declined
79. Invited Speaker, "Electronic Structure And Reactivity in the Condensed Phase", Physical Chemistry Colloquium, Department of Chemistry, University of Notre Dame, August 1999
80. Invited Speaker, "Theoretical Characterization of Electronic Structure And Reactivity in The Condensed Phase", Department of Chemistry, University of Alberta, Edmonton, Canada, November 1999
81. Invited Speaker, "Electronic Structure And Reactivity in The Condensed Phase: Computational Studies", Physical Chemistry Seminar, Department of Chemistry, University of Washington, Seattle, WA, March 2000

82. Invited Speaker, "Electronic Structure and Reactivity in The Condensed Phase: Computational Studies", Symposium on "Potential Energy Surfaces: From Polyatomics to Macromolecules", 219-th ACS Meeting, San Franscico, March 2000; also Session Chair.
83. Invited Speaker, "Recent Research on Electronic Structure and Reactivity in the Aqueous Phase", University of Kyoto, October 2000.
84. Invited Speaker, "Recent Research on Electronic Structure and Reactivity in the Aqueous Phase", University of Tokyo, October 2000.
85. Poster Presentation, "A Temperature-Dependent Ozonolysis Study of Ethene and Propene, AGU Fall Meeting, November 2000.
86. Invited Speaker, "Computational Approaches for Nanoscience", University of Tokyo, February 2001.
87. Invited Speaker, "Computational Approaches for Nanoscience", 4th International Symposium on Intermaterials, University of Osaka, February 6-7, 2001.
88. Invited Speaker, "Towards ab initio Cavities for Dielectric Continuum Models of Solvation", 4th International Congress of Theoretical Chemical Physics, Marly-le-Roi, France, July 9-16, 2002.
89. Invited Speaker, "Towards ab initio Cavities for Dielectric Continuum Models of Solvation", 224th ACS National Meeting, Symposium on :"Classical and Quantum Statistical Mechanics Studies of Solvation", Boston, Aug. 18-22, 2002.
90. Invited Speaker, "Towards ab initio Cavities for Dielectric Continuum Models of Solvation", ESPA2002 "Electronic Structure Principles and Applications", Sevilla, Spain, Sept. 11-13, 2002.
91. Invited Speaker, "Computational Studies of Complex Systems: Application to Aqueous Solvation and Biochemistry", Physical Chemistry Colloquium, Department of Chemistry, University of Sherbrooke, Sherbrooke, Canada, Oct. 31, 2002.
92. Invited Speaker, "Advances for Dielectric Continuum Models of Solvation", Physical Chemistry Department Seminar, University of Hiroshima, Hiroshima, Japan, Dec. 4, 2002.
93. Invited Speaker, "Integrals, Methods, and Applications: Electron Transport in Oxides", Symposium in Honor of Vic Saunders on Molecular and Solid State Quantum Chemistry, Daresbury, England, June 2003.
94. Invited Speaker, "Nano-Tailored Reactivity: Models, Tools, and Examples", Workshop on Computational Nanoscience, Argonne National Laboratory, Aug. 2003.
95. Invited Speaker, "Chimie Theorique et Outils Informatiques: Quel Avenir ?", International Congress of Theoreticians of Latin Speaking Countries, Marrakech, Morroco, Sept. 2003.
96. Invited Speaker, "Electronic Structure and Reactivity in Solution: Illustration of the QM/MM-pol-vib and Dielectric Continuum Models for Excited States and Dissociative Electron Attachment ", ITAMP Workshop on "Interaction of Slow Electrons with Molecular Solids and Biomolecules", Harvard-Smithsonian Center for Astrophysics, Cambridge MA, October 2003.
97. Invited Seminar Speaker, "Quantum Chemical Studies Relevant to Biochemistry: Electron Transfer in Ifc_3 Cytochrome and Clustered Damages in DNA", Center for Quantum Life Sciences, Hiroshima University, Hiroshima, Japan, Nov. 2003.
98. Invited Speaker, "Charge Transport in Metal Oxides", International Symposium on "theory and Application of Quantum Chemistry" in Honor of H.F. Schaefer Jr., Gyeongiu, Korea, Feb. 2004.
99. Invited Speaker, "Quasi-Classical ab initio direct dynamics for spectroscopy and reactivity", Truhlar's meeting on Computational Chemical Dynamics, Minneapolis, Oct. 2004.
100. Invited Speaker, "Theoretical Studies in Chemical Physics", Department of Chemistry, Univ. Hiroshima, Jan. 2005.
101. Invited Speaker, "Charge Transport in Metal Oxides: Theoretical Studies", Department of Chemistry, Univ. Hiroshima, Jan. 2005.
102. Invited Speaker, "Theoretical Studies in Chemical Physics", Department of Chemistry, Univ. of Tokyo, Jan. 2005.
103. Invited Speaker, "Charge Transport in Metal Oxides: Theoretical Studies", Sanibel Symposium, Mar. 2005.
104. Invited Speaker, "Charge Transport in Metal Oxides: Theoretical Studies", Chemistry Department, Argonne National Laboratory, Apr. 2005.
105. Invited Speaker, "Theoretical Investigation of Processes in the Radiolysis of Complex Aqueous Media", Pacifichem conference, Honolulu, Dec. 2005.
106. Invited Speaker, "Investigation of Radical Reactivity in Aqueous Media", Pacifichem Conference, Honolulu, Dec. 2005.
107. Invited Speaker, "Charge Transport in Metal Oxides: Theoretical Studies", International Congress of Quantum Chemistry (ICQC), Koyto, May 2006.

108. Invited Speaker, “Simulation for Proton Transfer and Transport in Conducting Polymer Membranes”, Invited presentation, Proton Solvation and Transport in Chemistry, Biology, and Materials Science, Herndon, VA, June 26, 2006.
109. Invited Speaker, “Charge Transport in Metal Oxides: Theoretical Studies”, Department of Chemistry, Hiroshima University, Sept. 2006
110. Invited Speaker, “Theoretical Investigation of Processes in the Radiolysis of Complex Aqueous Media”, Condensed Phase Interfacial and Molecular science Contractor’s meeting, Washington D.C. Oct. 2006.
111. Contributed Speaker, “Charge Transport in Metal Oxides: Theoretical Studies”, International Workshop On Oxide Surfaces (IWOX V), Lake Tahoe, Jan. 2007.
112. Invited Speaker, “Theoretical Studies of Charge Transport in Oxides”, Symposium in honor of W. A. Lester Jr., University of California, Berkeley, March 2007.
113. Invited Speaker, “Charge Transfer, Transport, and Reactivity in Complex Molecular Environments: Theoretical Studies for the Hydrogen Fuel Initiative”, BES Contractors' Meeting and DOE EERE HFI Technical Program Merit Review, Germantown, MD, May 14, 2007.
114. Invited Speaker, “Proton Exchange Membrane under Low Hydration Level: Insights from Atomistic Simulations and Electronic Structure Computations”, 58th Annual Meeting of the International Society of Electrochemistry, Banff, Canada, Sept. 2007.
115. Invited Speaker, “Charge Transfer, Transport, and Reactivity in Complex Molecular Environments”, Hiroshima University, Hiroshima, Japan, Jan. 2008.
116. Invited Speaker, “Charge Transfer, Transport, and Reactivity in Complex Molecular Environments: Theoretical Studies for the Hydrogen Fuel Initiative”, National Institute of Advanced Industrial Science and Technology AIST, Tsukuba, Japan, Jan. 2008.
117. Invited Speaker, “Proton Exchange Membrane under Low Hydration Level: Insights from Atomistic Simulations and Electronic Structure Computations”, Invited speaker, Symposium on Materials for Energy Conversion at the 2008 CSC meeting in Edmonton, Canada, May 2008.
118. Invited Speaker, “Charge Transport in Metal Oxides: a multi-scale simulation framework”, 1st Intl Conference of the Grand Challenge to Next-Generation Integrated Nanoscience, Tokyo, Japan, Jun. 2008.
119. Invited Speaker, “A new Charge-Dependent Solvation model”, International Symposium in Honor of Professor Ernest R. Davidson, 6th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), Vancouver BC, Jul. 2008.
120. Invited Speaker, “Charge Transport in Metal Oxides: Theoretical Studies”, Eighth Congress of the World Association of Theoretical and Computational Chemists (WATOC), Sydney, Australia, Sept. 2008.
121. Invited Speaker, “Proton Exchange Membrane under Low Hydration Level: Insights from Atomistic Simulations and Electronic Structure Computations”, Conference on Theory and Applications of Computational Chemistry (TACC), Shanghai, China, Sept. 2008.
122. Invited Speaker, “Charge Transport in Metal Oxides: a multi-scale simulation framework”, Joint ICTP-KFAS Workshop on Nanoscience for Solar Energy Conversion", International Centre for Theoretical Physics ICTP, Trieste, Italy, Oct. 2008.
123. Invited speaker, Colloquium, Department of Physics, (Computational Solid State Theory and Materials Science group), Michigan Technical University, Houghton, MI, Oct. 2009.
124. Invited speaker, colloquium, Department of Materials Science and Engineering College of Engineering and Center for Advanced Scientific Computing and Modeling (CASCaM) University of North Texas, Denton TX, Nov. 2009.
125. Invited speaker, Department of Chemistry, Waseda University, Waseda, Japan, “Theory and Simulations in Use-Inspired Applications for New Energy”, Dec. 2009.
126. Invited speaker, Department of Chemistry, Hiroshima University, Hiroshima, Japan, “Theories and Methods in Computational Chemistry”, Dec. 2009.
127. Invited speaker, QuLiS Institute, symposium on “Education Program for Innovative Research”, Hiroshima University, Hiroshima, Japan, “Theory and Simulations in Use-Inspired Applications for New Energy”, Dec. 2009.
128. Contributed Speaker, “Charge Transport in Metal Oxides: Theoretical Studies”, International Workshop on Oxide Surfaces (IWOX VII), Japan, Jan. 2010.
129. Invited speaker, symposium in the honor of Prof. H.F. King, Department of Chemistry, State University of New York, Buffalo, NY, May 2010.
130. Invited session chair, Department of Chemistry, symposium in the honor of Prof. J.M. Andre, Universite de Namur, Namur, BEL, Jul. 2010.
131. Invited speaker, 17th Canadian Symposium on Theoretical Chemistry, Edmonton, CA, July 2010.

132. Invited participant, Fifteenth International Workshop on Quantum Systems in Chemistry and Physics, Cambridge, UK, Aug. 2010.
133. Invited speaker, University College of London, workshop on 'Energy materials: electro- and photo-chemical interfaces and devices', Sept. 7-9, 2010. (declined)
134. Invited speaker, Centre Europeen de Calculs Atomics and Moleculaires (CECAM) workshop, "Titania for all seasons: Multi-functionality of an undercover semiconductor", T. Frauenheim organizer, Bremen, Germany, Sept. 2010.
135. Contributed speaker, Gordon Research Conference "Renewable Energies: Solar Fuels", Ventura CA, Jan. 2011.
136. Invited speaker, Department of Chemistry, Department Seminar, Washington State University, Pullman, WA, Feb. 2011.
137. Invited speaker, ACS National Spring Meeting, symposium in the honor of T. H. Dunning Jr., Annaheim, CA, Mar. 2011.
138. Invited speaker, International Conference on Computational and Experimental Engineering and Sciences, Nanjing, China, April, 2011 (declined).
139. Contributed speaker, Congress of the World Association of Theoretically Oriented Chemists WATOC 2011, Santiago de Compostella, Spain, Jul. 2011.
140. Invited Speaker, 7th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VII), Waseda University, Tokyo, Japan, Sept. 2011.
141. M. Dupuis, invited speaker, CECAM workshop on "when photo- meets electro-catalysis", Delmenhorst Germany, T. Frauenheim organizer, Oct. 4-7, 2011.
142. M. Dupuis, invited speaker, DOE workshop CCR/BES on CO2, org. D. L. DuBois, Annapolis MD, Oct 24-26, 2011
143. M. Dupuis, speaker, PNNL/TYC workshop, London UK, Nov. 1-3, 2011.
144. M. Dupuis, speaker, EFRC Review, Denver CO, Feb. 2012.
145. M. Dupuis, invited speaker, TYC workshop on Electron Transport, London, UK, June, 2012.
146. M.Dupuis, invited Speaker, 3d International Symposium on "Theory and Applications of Computational Chemistry, Pavia, Italy, Sept. 2012.
147. M. Dupuis, invited speaker, Department of Chemistry, University of Montpellier, France, Sept. 2012.
148. M. Dupuis, invited speaker, CECAM workshop on CO2, Bremen, Germany, Oct. 2012.
149. M. Dupuis**,** invited speaker, AIChE conference, Pittsburg OH, Oct 28, Nov. 1, 2012.
150. M. Dupuis**,** invited speaker, Mesilla workshop, org. W. Hase, Feb. 9-13, 2013
151. M. Dupuis**,** invited speaker, ACS National Meeting, Dan DuBois symposium, New Orleans LA, Apr., 2013
152. M. Dupuis, invited speaker, Molecular Quantum Mechanics 2013 in honor of Prof. Bartlett, Lugano SW, June 2013.
153. M. Dupuis**,** invited speaker, University of California at Santa Barbara, workshop on catalysis, Aug. 27-30, 2013
154. M. Dupuis, speaker, European Congress on Catalysis EUROPACAT 2013, Lyon FR, Sept. 2013
155. M. Dupuis, invited speaker, University of Saskatchewan, Edmonton CA, and University of Calgary CA, department seminar, Nov. 2013.
156. M. Dupuis, invited speaker, Symposium on Quantum Systems in Chemistry, Physics, and Biology QSCP 2013, Paraty, Brazil, Dec. 2013.
157. M. Dupuis, invited speaker, University of Tsinghua, Beijing, China, symposium in honor of Prof. J.M. Andre, Mar. 2014.
158. M. Dupuis, invited speaker, Department of Chemistry, Brookhaven National Laboratory, Upton, NY, April 2014.
159. M. Dupuis, invited speaker, Department of Chemical and Biological Chemistry, SUNY Buffalo, Buffalo, NY, May 2014.
160. M. Dupuis, invited speaker, International Chemical Congress of the Pacific Basin Societies (Pacifichem), December 2015.
161. M. Dupuis, invited speaker, Department of Chemistry, Worcester Polytechnic Institute, Worcester, MA, March September 2016
162. M. Dupuis, invited speaker, 8th Conference on Molecular Quantum Mechanics (MQM 2016), Uppsala, Sweden, June 2016
163. M. Dupuis, invited speaker, 2nd Symposium of "Advanced Lectures on Fundamentals for Solar Energy Conversion: Theory and Experiments", C. Li organizer, Dalian National Laboratory for Clean Energy, Dalian, China, July 2017.
164. M. Dupuis, invited speaker, 254th ACS National Meeting, symposium in honor of Peter Pulay, Washington DC, August 2017.
165. M. Dupuis, invited speaker, 58th Sanibel Symposium, St Simons Island, GA, USA, February 2018.

166. M. Dupuis, invited speaker, 256th ACS National Meeting, symposium on "Computational Photocatalysis", Boston, August 2018.
167. M. Dupuis, invited speaker, The 6th International Symposium on Solar Fuels and Solar Cells, Dalian National Laboratory for Clean Energy, Dalian, China, October 2018.
168. M. Dupuis, invited speaker, 2019 MRS Fall Meeting, Symposium on "Materials Science for efficient Water Splitting", Boston, December 2019.
169. M. Dupuis, speaker, 2020 WATOC meeting, Ruedenberg's Symposium, Vancouver BC, August 2020.
170. M. Dupuis, invited speaker, 5th International Symposium on "Theory and Applications of Computational Chemistry, Hokkaido University, Sapporo, Japan, Italy, Sept. 2020.