

List of Publication

So Hirata
July 27, 2004

Refereed articles

1. S. Hirata, H. Yoshida, H. Torii, and M. Tasumi,
The Journal of Chemical Physics, **103**, 8955–8963 (1995),
“Vibrational analyses of *trans,trans*-1,3,5,7-octatetraene and all-*trans*-1,3,5,7,9-decapentaene based on *ab initio* molecular orbital calculations and observed infrared and Raman spectra.”
2. S. Hirata, H. Torii, and M. Tasumi,
The Journal of Chemical Physics, **103**, 8964–8979 (1995),
“Vibrational analyses of *trans*-polyacetylene based on *ab initio* second-order Møller–Plesset perturbation calculations of *trans*-oligoenes.”
3. S. Hirata, H. Torii, Y. Furukawa, M. Tasumi, and J. Tomkinson,
Chemical Physics Letters, **261**, 241–245 (1996),
“Inelastic neutron scattering from *trans*-polyacetylene.”
4. S. Hirata, H. Torii, and M. Tasumi,
The Bulletin of the Chemical Society of Japan, **69**, 3089–3106 (1996),
“Stereostructural and vibrational analyses of *cis*-polyacetylene based on density functional calculations of oligoenes.”
5. S. Hirata and S. Iwata,
The Journal of Chemical Physics, **107**, 10075–10084 (1997),
“Density functional crystal orbital study on the normal vibrations of polyacetylene and polymethineimine.”
6. S. Hirata and S. Iwata,
The Journal of Chemical Physics, **108**, 7901–7908 (1998),
“Density functional crystal orbital study on the normal vibrations and phonon dispersion curves of all-*trans* polyethylene.”
7. S. Hirata and S. Iwata,
The Journal of Molecular Structure (Theochem) (Special issue for Professor Shigeru Huzinaga), **451**, 121–134 (1998),
“Analytical second derivatives in *ab initio* Hartree–Fock crystal orbital theory of polymers.”
8. S. Hirata, H. Torii, and M. Tasumi,
Physical Review B, **57**, 11994–12001 (1998),
“Density-functional crystal orbital study on the structures and energetics of polyacetylene isomers.”
9. S. Hirata and S. Iwata,
The Journal of Chemical Physics, **109**, 4147–4155 (1998),
“Analytical energy gradients in second-order Møller–Plesset perturbation theory for extended systems.”
10. S. Hirata and S. Iwata,
The Journal of Physical Chemistry A, **102**, 8426–8436 (1998),
“*Ab initio* Hartree–Fock and density functional studies on the structures and vibrations of an infinite hy-

drogen fluoride polymer.”

11. S. Hirata and M. Head-Gordon,
Chemical Physics Letters, **302**, 375–382 (1999),
“Time-dependent density functional theory for radicals: An improved description of excited states with substantial double excitation character.”

12. S. Hirata and M. Head-Gordon,
Chemical Physics Letters, **314**, 291–299 (1999),
“Time-dependent density functional theory within the Tamm–Dancoff approximation.”

13. S. Hirata, T. J. Lee, and M. Head-Gordon,
The Journal of Chemical Physics, **111**, 8904–8912 (1999),
“Time-dependent density functional study on the electronic excitation energies of polycyclic aromatic hydrocarbon radical cations of naphthalene, anthracene, pyrene, and perylene.”

14. S. Hirata, M. Head-Gordon, and R. J. Bartlett,
The Journal of Chemical Physics, **111**, 10774–10786 (1999),
“Configuration interaction singles, time-dependent Hartree–Fock, and time-dependent density functional theory for the electronic excited states of extended systems.”

15. S. Ivanov, S. Hirata, and R. J. Bartlett,
Physical Review Letters, **83**, 5455–5458 (1999),
“Exact exchange treatment for molecules in finite-basis-set Kohn–Sham theory.”

16. S. Hirata and R. J. Bartlett,
The Journal of Chemical Physics, **112**, 7339–7344 (2000),
“Many-body Green’s-function calculations on the electronic excited states of extended systems.”

17. S. Hirata and R. J. Bartlett,
Chemical Physics Letters, **321**, 216–224 (2000),
“High-order coupled-cluster calculations through connected octuple excitations.”

18. S. Hirata, M. Nooijen, and R. J. Bartlett,
Chemical Physics Letters, **326**, 255–262 (2000),
“High-order determinantal equation-of-motion coupled-cluster calculations for electronic excited states.”

19. J. Kong, C. A. White, A. I. Krylov, D. Sherrill, R. D. Adamson, T. R. Furlani, M. S. Lee, A. M. Lee, S. R. Gwaltney, T. R. Adams, C. Ochsenfeld, A. T. B. Gilbert, G. S. Kedziora, V. A. Rassolov, D. R. Maurice, N. Nair, Y. Shao, N. A. Besley, P. E. Maslen, J. P. Dombroski, H. Daschel, W. Zhang, P. P. Korambath, J. Baker, E. F. C. Byrd, T. Van Voorhis, M. Oumi, S. Hirata, C.-P. Hsu, N. Ishikawa, J. Florian, A. Warshel, B. G. Johnson, P. M. W. Gill, M. Head-Gordon, and J. A. Pople,
The Journal of Computational Chemistry, **21**, 1532–1548 (2000),
“Q-Chem 2.0: A high performance *ab initio* electronic structure program package.”

20. S. Hirata, M. Nooijen, and R. J. Bartlett,
Chemical Physics Letters, **328**, 459–468 (2000),
“High-order determinantal equation-of-motion coupled-cluster calculations for ionized and electron-attached states.”

21. C.-P. Hsu, S. Hirata, and M. Head-Gordon,

- The Journal of Physical Chemistry A*, **105**, 451–458 (2001),
“Excitation energies from time-dependent density functional theory for linear polyene oligomers: Butadiene to decapentaene.”
22. S. Hirata, M. Nooijen, I. Grabowski, and R. J. Bartlett,
The Journal of Chemical Physics, **114**, 3919–3928 (2001); Erratum **115**, 3967–3968 (2001),
“Perturbative corrections to coupled-cluster and equation-of-motion coupled-cluster energies: A determinantal analysis.”
23. M. Tobita, S. Hirata, and R. J. Bartlett,
The Journal of Chemical Physics, **114**, 9130–9141 (2001),
“A crystalline orbital study of polydiacetylenes.”
24. S. Hirata, S. Ivanov, I. Grabowski, R. J. Bartlett, K. Burke, and J. D. Talman,
The Journal of Chemical Physics, **115**, 1635–1649 (2001),
“Can optimized effective potentials be determined uniquely?”
25. S. Hirata, I. Grabowski, M. Tobita, and R. J. Bartlett,
Chemical Physics Letters, **345**, 475–480 (2001),
“Highly accurate treatment of electron correlation in polymers: Coupled-cluster and many-body perturbation theories.”
26. S. Ivanov, S. Hirata, and R. J. Bartlett,
The Journal of Chemical Physics, **116**, 1269–1276 (2002),
“Finite-basis-set optimized effective potential exchange-only method.”
27. I. Grabowski, S. Hirata, S. Ivanov, and R. J. Bartlett,
The Journal of Chemical Physics, **116**, 4415–4425 (2002),
“*Ab initio* density functional theory: OEP-MBPT(2)—a new orbital-dependent correlation functional.”
28. J. Szczepanski, J. Banisaukas, M. Vala, S. Hirata, R. J. Bartlett, and M. Head-Gordon,
The Journal of Physical Chemistry A, **106**, 63–73 (2002),
“Vibrational and electronic spectroscopy of the fluorene cation.”
29. S. Hirata, S. Ivanov, I. Grabowski, and R. J. Bartlett,
The Journal of Chemical Physics, **116**, 6468–6481 (2002) [selected as an article in *Virtual Journal of Biological Physics Research*, **3** (2002)],
“Time-dependent density functional theory employing optimized effective potentials.”
30. J. Szczepanski, J. Banisaukas, M. Vala, and S. Hirata,
The Journal of Physical Chemistry A, **106**, 6935–6940 (2002),
“Preresonance Raman spectrum of the C₁₃H₉ fluorene-like radical.”
31. S. Ivanov, S. Hirata, I. Grabowski, and R. J. Bartlett,
The Journal of Chemical Physics, **118**, 461–470 (2003).
“Connection between Görling–Levy and many-body perturbation approaches in density functional theory.”
32. J. Banisaukas, J. Szczepanski, J. Eyler, M. Vala, S. Hirata, M. Head-Gordon, J. Oomens, G. Meijer, and G. von Helden,
The Journal of Physical Chemistry A, **107**, 782–793 (2003),
“Vibrational and electronic spectroscopy of acenaphthylene and its cation.”

33. M. Tobita, S. Hirata, and R. J. Bartlett,
The Journal of Chemical Physics, **118**, 5776–5792 (2003),
“The analytical energy gradient scheme in the Gaussian based Hartree–Fock and density functional theory for two-dimensional systems using fast multipole method.”
34. S. Hirata, M. Head-Gordon, J. Szczepanski, and M. Vala,
The Journal of Physical Chemistry A, **107**, 4940–4951 (2003),
“Time-dependent density functional study of the electronic excited states of polycyclic aromatic hydrocarbon radical cations.”
35. S. Hirata,
The Journal of Physical Chemistry A, **107**, 9887–9897 (2003),
“Tensor contraction engine: abstraction and automated parallel implementation of configuration-interaction, coupled-cluster, and many-body perturbation theories.”
36. S. Hirata, C.-G. Zhan, E. Aprà, T. Windus, and D. A. Dixon,
The Journal of Physical Chemistry A, **107**, 10154–10158 (2003),
“A new, self-contained asymptotic correction scheme to exchange-correlation potentials for time-dependent density functional theory.”
37. Y. Asai, S. Hirata, and K. Yamashita,
The Journal of the Physical Society of Japan, **72**, 3286–3290 (2003),
“Local electronic excitation mechanism for nanofabrication of polydiacetylene molecular wire.”
38. S. Hirata, R. Podszwa, M. Tobita, and R. J. Bartlett,
The Journal of Chemical Physics **120**, 2581–2592 (2004),
“Coupled-cluster singles and doubles for extended systems.”
39. S. Hirata, T. Yanai, W. A. de Jong, T. Nakajima, and K. Hirao,
The Journal of Chemical Physics **120**, 3297–3310 (2004),
“Third-order Douglas–Kroll relativistic coupled-cluster theory through connected single, double, triple, and quadruple substitutions: Applications to diatomic and triatomic hydrides.”
40. J. Banisaukas, J. Szczepanski, J. Eyler, M. Vala, and S. Hirata,
The Journal of Physical Chemistry A **108**, 3713–3722 (2004),
“Vibrational and electronic absorption spectroscopy of 2,3-benzofluorene and its cation. Photodissociation pathways of the cation.”
41. S. Hirata,
The Journal of Chemical Physics **121**, 51–59 (2004),
“Higher-order equation-of-motion coupled-cluster methods.”
42. R. J. Bartlett, I. Grabowski, S. Hirata, and S. Ivanov,
The Journal of Chemical Physics (in press),
“The exchange-correlation potential in *ab initio* density functional theory.”
43. S. Hirata, M. Valiev, M. Dupuis, S. S. Xantheas, S. Sugiki, and H. Sekino,
Molecular Physics (Special Issue for Professor Rodney J. Bartlett) (submitted),
“Fast electron correlation methods for molecular clusters in the ground and excited states.”

44. S. Hirata, P.-D. Fan, A. A. Auer, M. Nooijen, and P. Piecuch,
The Journal of Chemical Physics (submitted),
“Automated derivation and parallel implementation of combined coupled-cluster and many-body perturbation theories.”

Proceedings of International Conferences

1. G. Baumgartner, D. E. Bernholdt, D. Cociorva, R. Harrison, S. Hirata, C.-C. Lam, M. Nooijen, R. Pitzer, J. Ramanujam, and P. Sadayappan,
Proceedings of Supercomputing 2002 (2002),
“A high-level approach to synthesis of high-performance codes for quantum chemistry.”

2. M. Vala, J. Szczepanski, J. Banisaukas, and S. Hirata,
NASA Laboratory Astrophysics Workshop 2002 (2002),
“Dehydrogenated neutral PAH radicals as carriers of the DIBs? Spectroscopy of the fluorene-like C₁₃H₉ radical.”

3. T. L. Windus, E. J. Bylaska, M. Dupuis, S. Hirata, L. Pollack, D. M. Smith, T.P. Straatsma, and E. Aprà,
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),
“NWChem: New functionality.”

4. T. Yanai, H. Nakano, T. Nakajima, T. Tsuneda, S. Hirata, Y. Kawashima, Y. Nakao, M. Kamiya, H. Sekino, and K. Hirao,
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),
“UTChem — A program for *ab initio* quantum chemistry.”

Book Chapters

1. S. Hirata,
Encyclopedia for Experimental Chemistry, 5th Edition, (The Chemical Society of Japan, 2003),
“Density functional theory”, a chapter in the volume of “Computational chemistry” (in Japanese).

Poster Presentation in International Conferences

1. S. Hirata and S. Iwata,
Fukuoka Conference on Theoretical Chemistry: From Atoms to Clusters (1997),
“Density functional crystal orbital study on the normal vibrations of polyacetylene and polymethineimine.”

2. S. Hirata and S. Iwata,
The 38th Sanibel Symposium (1998),
“Analytical first and second derivatives in *ab initio* crystal orbital theory.”

3. S. Hirata and S. Iwata,
The 13th Canadian Symposium on Theoretical Chemistry (1998),
“Development and application of analytical energy gradient methods in correlated crystal orbital theories.”

4. S. Hirata and M. Head-Gordon,

The 39th Sanibel Symposium (1999),
“Time-dependent density functional theory for radicals: An improved description of excited states with substantial double excitation character.”

5. S. Hirata and R. J. Bartlett,
The 40th Sanibel Symposium (2000),
“High-order configuration interaction, many-body perturbation, and coupled cluster calculations.”

6. S. Hirata, M. Nooijen, and R. J. Bartlett,
Symposium in Memory of Michael C. Zerner (2000),
“A determinantal coupled-cluster method.”

7. S. Hirata, S. Ivanov, K. Burke, I. Grabowski, J. D. Talman, and R. J. Bartlett,
The 41st Sanibel Symposium (2001),
“Can optimized effective potentials be determined uniquely?”

8. S. Hirata, M. Nooijen, I. Grabowski, and R. J. Bartlett,
A Symposium on Frontiers of Theoretical Chemistry (2001),
“Determinant-based coupled-cluster methods.”

9. S. Hirata, S. Ivanov, I. Grabowski, and R. J. Bartlett,
The 42nd Sanibel Symposium (2002),
“Ab initio DFT for excited states: time-dependent OEP.”

10. S. Hirata, G. Baumgartner, D. E. Bernholdt, D. Corciorva, R. J. Harrison, M. Nooijen, R. Pitzer, J. Ramanujam, P. Sadayappan, and J. W. Wilkins,
2002 American Conference on Theoretical Chemistry (2002),
“Operator and tensor contraction engines — computer aided synthesis of coupled-cluster programs of any given excitation order.”

Invited Talks in Conferences

1. S. Hirata,
The 65th Okazaki Conference (2000),
“The CIS, TDHF, TDDFT, and MBGF approaches to the electronic excited states of extended systems.”

2. S. Hirata,
A Symposium on Frontiers of Theoretical Chemistry (2001),
“Toward *ab initio* density functional theory.”

3. S. Hirata,
A CECAM Workshop: Rigorous ab-initio studies of periodic systems: approaches to electron correlation (2003),
“POLYMER: a crystalline orbital program.”

4. S. Hirata,
226th National American Chemical Society Meeting (2003),
“Artificial intelligence for electronic structures: automated parallel implementations of configuration-interaction, coupled-cluster, and many-body perturbation theories.”

5. S. Hirata,

44th Sanibel Symposium (2004),
“First-principle quantum chemical calculations of polymers.”

6. S. Hirata,
The Systematic Treatment of Electron Correlation: A Celebration of the Science of Rodney J. Bartlett (2004),
“Science with R. J. Bartlett—extended systems, *ab initio* DFT, coupled-cluster theory.”

7. S. Hirata,
Asian Pacific Conference on Theoretical & Computational Chemistry (2004),
“Artificial intelligence for electronic structure: automated derivation and parallel implementation of CI, CC, and MBPT.”

Invited lectures

1. S. Hirata
University of Tokyo (Tokyo, 2003),
“Artificial intelligence for electronic structure.”

2. S. Hirata,
Seminar, Department of Chemistry, University of Florida (Gainesville, 2003),
“‘Computational’ spectroscopy for molecules and polymers.”

3. S. Hirata,
Science at the Edge, Michigan State University (East Lansing, 2004),
“‘Computational’ spectroscopy for molecules and polymers.”

4. S. Hirata,
The National Institute for Advanced Industrial Science and Technology (Tsukuba, 2004),
“Artificial intelligence for electronic structure: automated derivation and implementation of many-electron theories.”

5. S. Hirata,
Toyohashi University of Technology (Toyohashi, 2004),
“Artificial intelligence for electronic structure: automated derivation and implementation of many-electron theories.”

6. S. Hirata,
Kyoto University (Kyoto, 2004),
“Artificial intelligence for electronic structure: automated derivation and implementation of many-electron theories.”

7. S. Hirata,
Society of Computer Chemistry (2004),
“Artificial intelligence for electronic structure: automated derivation and implementation of many-electron theories.”

Theses

1. A graduation thesis,
“Vibrational analyses of linear polyenes based on *ab initio* molecular orbital theory,”

The University of Tokyo (1994, in Japanese), Professor Mitsuo Tasumi (supervisor).

2. A master's thesis,

“Vibrational analyses of polyacetylene based on *ab initio* molecular orbital and density functional theory,”
The University of Tokyo (1996, in Japanese), Professor Mitsuo Tasumi (supervisor).

3. A doctoral thesis,

“Development and application of analytical derivative methods in *ab initio* crystal orbital theory,”
The Graduate University for Advanced Studies (1998), Professor Suehiro Iwata (supervisor).

Quantum Chemistry Computer Codes

1. “POLYMER 1.0,” S. Hirata, M. Tasumi, H. Torii, S. Iwata, M. Head-Gordon, and R. J. Bartlett, (1999).
A first-principles quantum chemistry computer program for infinite one-dimensional lattices (polymers). The ground-state energies (Hartree–Fock theory, density functional theory, second- and third-order many-body perturbation theory, and coupled-cluster theory), optimized geometries (analytical gradient method), vibrational frequencies, quasi-particle energies (second-order many-body perturbation theory and Green's function theory), excited-state energies (configuration interaction singles theory, time-dependent Hartree–Fock theory, and time-dependent density functional theory) can be calculated for polymers. For atoms and molecules, full configuration interaction calculations, high-order determinantal many-body perturbation calculations, high-order determinantal coupled-cluster calculations, high-order determinantal equation-of-motion coupled-cluster calculations, and optimized effective potential calculations can be performed.

2. “Q-CHEM 2.0,” J. Kong, C. A. White, A. I. Krylov, D. Sherrill, R. D. Adamson, T. R. Furlani, M. S. Lee, A. M. Lee, S. R. Gwaltney, T. R. Adams, C. Ochsenfeld, A. T. B. Gilbert, G. S. Kedziora, V. A. Rassolov, D. R. Maurice, N. Nair, Y. Shao, N. A. Besley, P. E. Maslen, J. P. Dombroski, H. Daschel, W. Zhang, P. P. Korambath, J. Baker, E. F. C. Byrd, T. Van Voorhis, M. Oumi, S. Hirata, C.-P. Hsu, N. Ishikawa, J. Florian, A. Warshel, B. G. Johnson, P. M. W. Gill, M. Head-Gordon, and J. A. Pople (2000).
A high-performance *ab initio* molecular orbital and density functional program package widely in use by academic and industrial research scientists throughout the world.

3. “NWCHEM 4.1,” R. J. Harrison, J. A. Nichols, T. P. Straatsma, M. Dupuis, E. J. Bylaska, G. I. Fann, T. L. Windus, E. Apra, W. de Jong, S. Hirata, M. T. Hackler, J. Anchell, D. Bernholdt, P. Borowski, T. Clark, D. Clerc, H. Dachsel, M. Deegan, K. Dyall, D. Elwood, H. Fruchtl, E. Glendenning, M. Gutowski, K. Hirao, A. Hess, J. Jaffe, B. Johnson, J. Ju, R. Kendall, R. Kobayashi, R. Kutteh, Z. Lin, R. Littlefield, X. Long, B. Meng, T. Nakajima, J. Nieplocha, S. Niu, M. Rosing, G. Sandrone, M. Stave, H. Taylor, G. Thomas, J. van Lenthe, K. Wolinski, A. Wong, and Z. Zhang (2002). Pacific Northwest National Laboratory, Richland, Washington 99352-0999, USA.

4. “TENSOR CONTRACTION ENGINE 1.0,” S. Hirata (2003). Pacific Northwest National Laboratory, Richland, Washington 99352-0999, USA.