

## Curriculum Vitae: So Hirata

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Departments of Chemistry and Physics  
Quantum Theory Project and Center for Macromolecular Science and Engineering  
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### Education

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- Ph.D. (1998) The Graduate University for Advanced Studies and Institute for Molecular Science (JSPS Research Fellow)
- M.Sc. (1996) The University of Tokyo
- B.Sc. (1994) The University of Tokyo

### Positions Held

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- **Assistant Professor**, Department of Chemistry, University of Florida, 2004–present.
- **Affiliate Assistant Professor**, Department of Physics, University of Florida, 2007–present.
- **Adjunct Associate Professor**, Hiroshima University, 2004–present.
- **Senior Research Scientist**, Pacific Northwest National Laboratory, 2001–2004.
- **Visiting Assistant in Postdoctoral Program**, University of Florida, 2000–2001.
- **Postdoctoral Research Associate**, University of Florida, 1999–2000.
- **Visiting Scholar**, University of California, Berkeley, 1998–1999.

### Awards

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- Japan Society for the Promotion of Science **Research Fellowship for Young Scientists**, 1996–99.
- University of Illinois, Urbana–Champaign, **MCC Travel Award**, 2005.
- **Hewlett–Packard Outstanding Junior Faculty Award**, ACS COMP and Hewlett–Packard Company, 2008.

### Research Interests

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First-principles many-electron theories and density functional theory for the electronic structure of atoms, molecules, and crystalline solids; high-performance parallel computing and domain-specific code generation for many-electron theories; coupled-cluster and many-body perturbation theories; excited-state electronic structure theories; anharmonic vibrational analysis; polycyclic aromatic hydrocarbons; conjugated conducting polymers.

### Teaching and Synergistic Activities

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- Co-organizer of annual Sanibel Symposia (St. Simons Island, GA).
- Member of NaBiT (Nano-Bio-Information Technology) Educational Program of Hiroshima University, Hiroshima, Japan.
- Co-author of the Q-CHEM, NWCHEM, and UTCHEM computational chemistry program suites and principal author of the POLYMER and TCE computational chemistry programs.
- Courses taught: Spring 2005, Spring 2006, Spring 2007, Fall 2007 CHM 4412 (4 credit hours) Physical Chemistry II: Quantum Mechanics and Spectroscopy; Fall 2005, Fall 2006 CHM 6490 (3 credit hours) Theoretical Molecular Spectroscopy.
- Graduate students supervised: Long Yu (2<sup>nd</sup> year), Murat Keceli (2<sup>nd</sup> year), and Toru Shiozaki (2<sup>nd</sup> year).
- Undergraduate student supervised: Nathan Tennyson (06–07) and Michael Chin (07–present).
- Postdoctoral associates supervised: Peng-Dong Fan (Ph.D. Michigan State Univ. 05–07), Muneaki Kamiya (Ph.D. Univ. Tokyo 05–07), Valerie Rodriguez-Garcia (Ph.D. UF 05–06).
- Judge of Lincoln Middle School Science Fair (January 2006).

## Selected Publications

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1. S. Hirata and S. Iwata, "Analytical energy gradients in second-order Møller–Plesset perturbation theory for extended systems," *The Journal of Chemical Physics* **109**, 4147–4155 (1998).
2. S. Hirata, M. Head-Gordon, and R. J. Bartlett, "Configuration interaction singles, time-dependent Hartree–Fock, and time-dependent density functional theory for the electronic excited states of extended systems," *The Journal of Chemical Physics* **111**, 10774–10786 (1999).
3. S. Hirata and R. J. Bartlett, "Many-body Green's-function calculations on the electronic excited states of extended systems," *The Journal of Chemical Physics* **112**, 7339–7344 (2000).
4. S. Hirata, R. Podeszwa, M. Tobita, and R. J. Bartlett, "Coupled-cluster singles and doubles for extended systems," *The Journal of Chemical Physics* **120**, 2581–2592 (2004).
5. S. Hirata, "Third- and fourth-order perturbation corrections to excitation energies from configuration interaction singles," *The Journal of Chemical Physics* **122**, 094105 (2005).
6. S. Ivanov, S. Hirata, and R. J. Bartlett, "Exact exchange treatment for molecules in finite-basis-set Kohn–Sham theory," *Physical Review Letters* **83**, 5455–5458 (1999).
7. S. Hirata, T. J. Lee, and M. Head-Gordon, "Time-dependent density functional study on the electronic excitation energies of polycyclic aromatic hydrocarbon radical cations of naphthalene, anthracene, pyrene, and perylene," *The Journal of Chemical Physics* **111**, 8904–8912 (1999).
8. S. Hirata, "Higher-order equation-of-motion coupled-cluster methods," *The Journal of Chemical Physics* **121**, 51–59 (2004).
9. S. Hirata, "Symbolic algebra in quantum chemistry," *Theoretical Chemistry Accounts* **116**, 2–17 (2006) (the special issue "New Perspective in Theoretical Chemistry").
10. S. Hirata, T. Yanai, R. J. Harrison, M. Kamiya, and P.-D. Fan, "High-order electron-correlation methods with scalar relativistic and spin-orbit corrections," *The Journal of Chemical Physics* **126**, 024104 (2007).

## Grant Supports

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- **U.S. Department of Energy**, Office of Basic Energy Sciences, DE-FG02-04ER15621 (2007–10) "Breakthrough Design and Implementation of Many-Body Electronic and Vibrational Theories," (PI) \$330,000.
- **U.S. Department of Energy**, Office of Basic Energy Sciences, DE-FG02-04ER15621 (2004–7) "Breakthrough Design and Implementation of Many-Electron Theories for Electron Correlation," (PI) \$349,998.
- **U.S. National Science Foundation**, Grant No. CHE-0450462 (2004–6) "ITR/AP Collaborative Research: Synthesis of High-Performance Algorithms for Electronic Structure Calculations," (co-PI) \$63,000.
- **University of Florida** Research Opportunity Incentive Seed Fund (2004–5) "Modern Theory for Correlated Nuclear Motions," (PI) \$32,571.

## Ph.D and Postdoctoral Advisors

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- Professor Suehiro Iwata, Institute for Molecular Science (thesis).
- Professor Rodney J. Bartlett, University of Florida (postdoc).
- Professor Martin Head-Gordon, University of California, Berkeley (postdoc).