CURRICULUM VITAE

Henryk A. Witek

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Education

Ph.D. Quantum Chemistry, University of Tokyo, Japan, 2002
Development and applications of multireference perturbation theory
Advisor: Kimihiko Hirao

M.S. Quantum Chemistry, Jagiellonian University, Cracow, Poland, 1996
Modeling spectra of non-rigid molecules
Advisor: Marek Pawlikowski

Employment

2008-present: Associate professor, Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu, Taiwan
Development of computational methods in quantum chemistry
Modeling chemical and physical properties of nanostructures
Computational assistance for experiments in chemical physics and physical chemistry

2005-2008: Assistant professor, Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu, Taiwan
Development of computational methods in quantum chemistry
Modeling chemical and physical properties of nanostructures
Development of numerical algorithm for linear algebra problems

2003-2005: Postdoctoral fellow, Department of Chemistry and Emerson Center for Scientific Computations, Emory University, Atlanta, Georgia
Development of semiempirical quantum chemistry methods
Modeling vibrational spectra of large molecules
Nanochemistry and nanophysics of large carbon clusters
Adiabatic potential energy surfaces for polyatomic molecules
Distributed parallel programming techniques in quantum chemistry
Advisor: Keiji Morokuma

Academic Collaborations

2009-2010: Short scientific visits (in total 3 months) in Quantum Chemistry Research Institute, Kyoto, Japan
Development of the exact wave function methodology for quantum chemical calculations: analysis of the singular structure of atomic wave functions, assessment of various two-

electron basis sets applicable to very accurate quantum mechanical calculations for the helium atom, further progress in solving exactly the Schrödinger equation for the helium atom.
Cooperation: Hiroshi Nakatsuji, Hiroyuki Nakashima

2008: Short scientific visit (1 month) in Bremen Center for Computational Material Science, University of Bremen, Germany

Relativistic parameterization for the SCC-DFTB method: deriving and coding the two-center integration routines for distance-dependent Fock and overlap matrix elements.
Cooperation: Thomas Frauenheim, Christof Köhler, Grzegorz Mazur, Marcus Elstner

2008: Short scientific visit (2 weeks) at Institute for Advanced Research and Department of Chemistry, Nagoya University, Nagoya, Japan

Modeling IR and Raman spectra of various carbon nanostructures.
Cooperation: Stephan Irle

2007: Short scientific visit (1 month) in Bremen Center for Computational Material Science, University of Bremen, Germany

Relativistic parameterization for the SCC-DFTB method: deriving and coding the two-center integration routines for distance-dependent Fock and overlap matrix elements.
Cooperation: Thomas Frauenheim, Christof Köhler

2006: Short scientific visit (2 weeks) in Department of Physical and Theoretical Chemistry, Technical University, Braunschweig, Germany

Development of the self-consistent charge density-functional tight-binding method
Cooperation: Marcus Elstner

2006: Short scientific visit (2 weeks) in Bremen Center for Computational Material Science,University of Bremen, Germany

Relativistic parameterization for the density-functional tight-binding method
Cooperation: Thomas Frauenheim, Christof Köhler

2004: Short scientific visit (1 month) in Department of Theoretical Physics, University of Paderborn, Germany

Development of the self-consistent charge density-functional tight-binding method
Cooperation: Marcus Elstner

2004-2005: Research projects, Department of Math and Computer Science, Emory University, Atlanta, Georgia

Surface-constrained global minimization of carbon nanoclusters
Distributed parallel implementation of the SCC-DFTB method
Cooperation: Dawid Kurzyniec, Vaidy Sunderam

2003: Short scientific visit (3 months) in Department of Chemistry, Korean Advanced Institute of Science and Technology, Daejon, South Korea

Development of relativistic Dirac-equation-based multireference perturbation theory
Advisor: Yoon-Sup Lee

2002: Short scientific visit (1 month) in Department of Chemistry, Jagiellonian University, Cracow, Poland

Modeling spectroscopic properties of tungsten oxide glasses
Advisor: Piotr Petelenz

2002: Short scientific visit (4 months) in Intelligent Modeling Laboratory, University of Tokyo, Japan

Development of optimal perturbative partitioning of many-body Hamiltonians
Cooperation: Haruyuki Nakano

1998: Short scientific visit (4 months) in Fritz Haber Center, Hebrew University, Jerusalem, Israel

Simulations of water layers deposited on metal surfaces
Advisor: Victoria Buch

1996-1997: Research project (1 year) in Quantum Chemistry Laboratory, University of Warsaw, Poland

Calculations for low-lying states of large organic molecules
Advisor: Lucjan Piela

1995: Tempus exchange program (5 months) in Department of Chemistry, University of Antwerp, Belgium

Electron microscopy of atmospheric nanoparticles
Advisor: René Van Grieken

Teaching experience

- General Chemistry I and II (undergraduate), Introduction to Numerical Analysis, Linear Algebra for Scientists, Quantum Chemistry, Computational Chemistry, Group Theory, 2005-2010, National Chiao Tung University, Hsinchu, Taiwan (in English)
- Computer Methods in Chemistry (TA), 2000-2002, University of Tokyo, Japan (in Japanese)
- Quantum Chemistry and Introduction to Physics (TA), 1996-1997, University of Warsaw, Poland (in Polish)

Honors and awards

- November 2009, Young Outstanding Scholar Award (年輕學者傑出研究獎), College of Science, National Chiao Tung University
- September 2006, Hewlett-Packard Outstanding Junior Faculty Award, 232th ACS meeting, Computers in Chemistry Section, San Francisco, USA
- 2005–2010, Young Faculty Award and Scholarship from the Foundation for the Advancement of Outstanding Scholarship, Taipei, Taiwan
- 1998–2002 MONBUSHO Research Scholarship, Japan
- 1995 European Union TEMPUS Fellowship

Invited talks

- May 2010, invited department talk, “Accuracy limits in quantum chemistry”, Institute of Atomic and Molecular Sciences, Taipei, Taiwan
- July 2009, invited speaker, “When finite becomes infinite…”, CREST International Symposium on Theory and Simulations of Complex Molecular Systems, Fukui Institute for Fundamental Chemistry, Kyoto, Japan

- March 2009, invited talk, "NgMX and MNgX: Are they stable?" and "Mn_2: A challenge for theory and experiment",13th East Asian Workshop on Chemical Dynamics, Taipei, Taiwan
- July 2008, keynote speaker, "When finite becomes infinite", Current Trends in Theoretical Chemistry V, Krakow, Poland
- April 2008, a contribution to invited talk, "Rovibronic bands of the $A^2B_2 \leftarrow X^2B_1$ transition of C_6H_5O and C_6D_5O detected with cavity ringdown absorption near 1.15-1.32 μm", C.-W. Cheng, H. A. Witek, and Y.-P. Lee, 235th ACS meeting, Division of Physical Chemistry, New Orleans, USA
- December 2007, invited talk, "How much can we trust quantum chemical calculations?", Joint Symposium on Computational Chemistry, Hanoi, Vietnam
- May 2007, invited talk: "The SCC-DFTB method: a powerful technique for computational simulations of large systems", 11th East Asian Workshop on Chemical Dynamics, Tokyo, Japan
- September 2006, invited talk, "Relativistic parameterization of the SCC-DFTB method", H. A. Witek, 232nd ACS meeting, Division of Computers in Chemistry, New Orleans, USA
- March 2005, a contribution to invited talk, "Analytical second derivatives, parameterization, and improvement of the DFTB (Density Functional Tight Binding) method", H. A. Witek, G. Zheng, D. G. Musaev, S. Irle, D. Quiñonero, M. Elstner, and K. Morokuma, 229th ACS meeting, Division of Computers in Chemistry, New Orleans, USA
- March 2005, a contribution to invited talk, "Density functional tight binding (DFTB) method and its application to molecular dynamics simulation of formation of fullerenes and carbon nanotubes", S. Irle, G. Zheng, H. A. Witek, K. Morokuma, and M. Elstner, 229th ACS meeting, Division of Fuel Chemistry, New Orleans, USA

Scientific publications

1. H. Witek and V. Buch, "Structure of ice multilayers on metals", *J. Chem. Phys.* **110**, 3168 (1999)
2. J. P. Finley and H. A. Witek, "Diagrammatic complete active space perturbation theory: Calculations on benzene, N_2, and LiF", *J. Chem. Phys.* **112**, 3958 (2000)
3. H. A. Witek, T. Nakajima, and K. Hirao, "Relativistic and correlated all-electron calculations on the ground and excited states of AgH and AuH", *J. Chem. Phys.* **113**, 8015 (2000)
4. Y.-K. Choe, H. A. Witek, J. P. Finley, and K. Hirao, "Identifying and Removing Intruder States in Multireference Møller-Plesset Perturbation Theory", *J. Chem. Phys.* **114**, 3913 (2001)
5. H. A. Witek, D. G. Fedorov, K. Hirao, A. Viel, and P.-O. Widmark, "Theoretical Study of the Unusual Potential Energy Curve of the $A^1\Sigma^+$ state of AgH", *J. Chem. Phys.* **116**, 8396 (2002)
6. H. A. Witek, Y.-K. Choe, J. P. Finley, and K. Hirao, "Intruder State Avoidance Møller-Plesset Perturbation Theory", *J. Comput. Chem.* **23**, 957 (2002)
7. H. A. Witek, N. Nakano, and K. Hirao, "Multireference Perturbation Theory with Optimized Partitioning. I. Theoretical and Numerical Aspects", *J. Chem. Phys.* **118**, 8197 (2003)
8. H. A. Witek, N. Nakano, and K. Hirao, "Multireference Perturbation Theory with Optimized Partitioning. II. Application to Molecular Systems", *J. Comput. Chem.* **24**, 1390 (2003)
9. T. Ampula, D. Kurzyniec, V. Sunderam, and H. A. Witek, "The Genetic Algorithm Population Pluglet for the H2O Metacomputing System", *International Conference on Computational Science 2004*, pp. 140-147
10. H. A. Witek, S. Irle, and K. Morokuma, "Analytical second-order geometrical energy derivatives of the self-consistent-charge density-functional tight-binding method", *J. Chem. Phys.* **121**, 5163 (2004)

11. H. A. Witek and K. Morokuma, "Systematic study of vibrational frequencies calculated with the self-consistent-charge density-functional tight-binding method", *J. Comput. Chem.* **25**, 1858 (2004)
12. H. A. Witek, K. Morokuma, and A. Stradomska, "Modeling vibrational spectra using the self-consistent-charge density-functional tight-binding method. I. Raman spectra", *J. Chem. Phys.* **121**, 5171 (2004)
13. H. A. Witek, K. Morokuma, and A. Stradomska, "Modeling vibrational spectra using the self-consistent-charge density-functional tight-binding method. II. Infrared spectra", *J. Theor. Comput. Chem.* **4**, 639 (2005)
14. E. Malolepsza, H. A. Witek, and K. Morokuma, "Accurate vibrational frequencies using the self-consistent-charge density-functional tight-binding method", *Chem. Phys. Lett.* **412**, 237 (2005)
15. X. Feng, S. Irle, H. A. Witek, K. Morokuma, R. Vidic, and E. Borguet, "Extreme Sensitivity of Ammonia Interaction with Single Walled Carbon Nanotube Bundles to the Presence of Defect Sites and Functionalities", *J. Am. Chem. Soc.* **127**, 10533 (2005)
16. E. Broclawik, A. Góra, P. Liguzinski, P. Petelenz, and H. Witek, "Quantum chemical modeling of electrochromism of tungsten oxide films", *J. Chem. Phys.* **124**, 054709 (2006)
17. H. A. Witek, S. Irle, G. Zheng, B. de Jong, and K. Morokuma "Modeling carbon nanostructures with the self-consistent charge density-functional tight-binding method: Vibrational and electronic spectra of C_{28}, C_{60}, and C_{70}", *J. Chem. Phys.*, **125**, 214706 (2006)
18. E. Malolepsza, H. A. Witek, S. Irle, "Comparison of Geometric, Electronic, and Vibrational Properties of small fullerenes C_{20}–C_{36}", *J. Phys. Chem. A*, **111**, 6649, (2007)
19. G. Zheng, H. A. Witek, P. Bobadova-Parvanova, S. Irle, D. Musaev, R. Prabhakar, K. Morokuma, "Parameter Calibration of Transition-Metal Elements for the Spin-Polarized Self-Consistent-Charge Density-Functional Tight-Binding (DFTB) Method: Sc, Ti, Fe, Co, and Ni", *J. Chem. Theor. Comp.*, **3**, 1349 (2007)
20. H. A. Witek, C. Koehler, T. Frauenheim, K. Morokuma, M. Elstner, "Relativistic Parametrization of the Self-Consistent-Charge Density-Functional Tight-Binding Method. 1. Atomic Wave Functions and Energies", *J. Phys. Chem. A*, **111**, 5712 (2007)
21. H. A. Witek, B. Trzaskowski, E. Małolepsza, K. Morokuma, and L. Adamowicz, "Computational study of molecular properties of aggregates of C_{60} and (16, 0) zigzag nanotube", *Chem. Phys. Lett.* **446**, 87 (2007)
22. Y.-J. Lu, L. Lee, J.-W. Pan, H. A. Witek, and J. J. Lin, "Dynamics of the F_2+CH_3SCH_3 reaction: A molecule-molecule reaction without entrance barrier", *J. Chem. Phys.* **127**, 101101 (2007)
23. C.W. Cheng, Y.P. Lee, and H. A. Witek, "Theoretical investigation of molecular properties of the first excited state of phenoxyl radical", *J. Phys. Chem. A*, 112, 2648 (2008)
24. Y.-J. Lu, L. Lee, J.-W. Pan, H. A. Witek, and J. J. Lin, "Barrierless reactions between two closed-shell molecules. I. Dynamics of F_2+CH_3SCH_3 reaction", *J. Chem. Phys.* 128, 104317 (2008)
25. C. Camacho, S. Yamamoto, and H. A. Witek, "Choosing a proper complete active space in calculations for transition metal dimers: Ground state of Mn_2 revisited", *Phys. Chem. Chem. Phys.* 10, 5128 (2008)
26. C.W. Cheng, Y.P. Lee, and H. A. Witek, "Theoretical investigation of molecular properties of the first excited state of thiophenoxyl radical", *J. Phys. Chem. A* **112**, 11998 (2008)
27. C.W. Cheng, H. A. Witek, and Y.P. Lee, "Rovibronic bands of the $A\ ^2B_2 \leftarrow X\ ^2B_1$ transition of C_6H_5O and C_6D_5O detected with cavity ringdown absorption near 1.2 μm", *J. Chem. Phys.* 129, 154307 (2008).
28. C.H. Mou and H.A. Witek, "Theoretical study of noble-gas containing metal halides", *J. Chem. Phys.* **129**, 244310 (2008)

29. C. Camacho, S. Yamamoto, and H. A. Witek, "Intruder states in multireference perturbation theory: ground state of Mn_2", *J. Comput. Chem.* **30**, 468-478 (2009)
30. E. Małolepsza, Y. P. Lee, H. A. Witek, S. Irle, C. F. Lin, and H. M. Hsieh, "Comparison of geometric, electronic, and vibrational properties for all pentagon/hexagon-bearing isomers of fullerenes C_{38}, C_{40}, and C_{42}", *Int. J. Quantum Chem.* **109**, 1999 (2009)
31. Y.-J. Wu, H.-F. Chen, C. Camacho, H. A. Witek, S.-C. Hsu, M.-Y. Lin, S.-L. Chou, J. F. Ogilvie, and B.-M. Cheng, "Formation and identification of interstellar molecule linear C_5H from photolysis of methane dispersed in solid neon", *Astrophys. J.* **701**, 8-11 (2009)
32. M. Gaus, C. P. Chou, H. A. Witek, M. Elstner, "Automatized parametrization of SCC-DFTB repulsive potentials: Application to hydrocarbons", *J. Phys. Chem. A*, 113, 11866-11881 (2009)
33. C. Camacho, R. Cimiraglia, and H. A. Witek, "Multireference perturbation theory can predict a false ground state", *Phys. Chem. Chem. Phys.* **12**, 5058–5060 (2010)
34. C. Camacho, H. A. Witek, and R. Cimiraglia, "The low-lying states of the scandium dimer", *J. Chem. Phys.* **132**, (2008), in press