STEPHAN IRLE

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PERSONAL

- Married, one child.
- Citizen of Germany.
- Permanent resident of Japan since February 29, 2012.
- Former permanent resident of the U.S.A., A# 095-237-730.

EDUCATION & TRAINING

- **Doctor of Philosophy**, March 17, 1997.
  Institute of Theoretical Chemistry and Radiation Chemistry, University of Vienna, Austria
  Thesis: *"Quantum chemical model studies on doped oligothiophenes and oligo(p-phenyls)"*
  Supervisor: Prof. Hans Lischka.
- **Master of Science** (Summa Cum Laude), September 30, 1992.
  Theoretical Chemistry, University of Siegen, Germany
  Thesis: *"Characterization of Atoms and Chemical Bonds in Molecules by Means of the Electron Density"*
  Supervisor: Prof. W. H. Eugen Schwarz.

AWARDS AND HONORS

- **Funded research contracts** from ACS-PRF, NSF, ONR, ORNL Laboratory Directed Research & Developed (LDRD) (U.S.A.); AC21, JSPS, JST, MEXT, NIFS (Japan), ERC (European Union); IAEA (United Nations); and DENSO Corporation (Japan).
- **Author Profile**, *Angew. Chem. Int. Ed.* Early View (2017). DOI: 10.1002/anie.201712472
- **Award** from the NanotechJapan Nanotechnology Platform: "Six Major Results of 2016 from Nanotechnology Platform Japan" (平成28年度利用6大成果賞) for: "The material development of liquid crystal glue that can be exfoliated by light even at high temperature" (高温でも使える、光ではがせる液晶接着材料の開発), February 17, 2017.
- **Adjunct Professorship**, Institute for Computational Science (IACS), Stony Brook University, Stony Brook, NY, U.S.A., October 2015 – September 2018.
- **Invited member** of the MEXT "Post-K computer" project "Development of the new fundamental technologies for highly efficient creation, conversion and storage, and use of energy", Institute for Molecular Science (IMS), Okazaki, Japan, April 2015 – March 2017.
- **Visiting Professorship**, Institute of Theoretical and Simulational Chemistry, Academy of Fundamental and Interdisciplinary Sciences, Harbin Institute of Technology, Harbin, China, December 2012.
- **Visiting Professorship**, Bremen Center for Computational Material Science (BCCMS), Bremen University, Germany, September 2012.
- **Visiting Professorship**, Fundamental Physics Simulation Research Division, National Institute for Fusion Science (NIFS), Gifu, Japan, April 2008 – March 2010.
- **Fukui Research Fellowship** from the Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, Japan, May – November 2006.
- **JSPS Short Term Visiting Fellowship** with Prof. Hisanori Shinohara (ID No. PE05031), Nagoya University, Nagoya, Japan, October – November 2005.

- **Travel Stipend** from the Division of Materials Research, NSF, for the 4th Workshop on Opportunities in Materials Theory (WOMT), Washington, DC, October 2004.
- **Visiting Fellowship** from the Establishment of the Austrian-Thai Centre for Computer-Assisted Chemical Education and Research (now named Computational Chemistry Unit Cell) at Chulalongkorn University, Bangkok, Thailand, October 1996.
- **Graduate Fellowship** from the University Foundation *"Chemical Reactivity and Molecular Order*", University of Siegen, Germany, January 1992 – September 1993.

EMPLOYMENT HISTORY

- **Computational Soft Matter Scientist**, Computational Sciences and Engineering Division & Chemical Science Division, Oak Ridge National Laboratory, U.S.A., May 2017 – present.
- **Principal Investigator**, Institute of Transformative Bio-Molecules (WPI-ITbM), Nagoya University, Japan, April 2013 – March 2017.
- **Professor of Chemistry**, Graduate School of Science, Nagoya University, Japan, April 2011 – March 2017.
- **Designated Associate Professor of Chemistry** (tenure track), Nagoya University, Japan, November 2006 – March 2011.
- **Fukui Fellow** (special faculty), Institute of Fundamental Chemistry Center, Kyoto University, Japan, May – October 2006.
- **Associate Scientist & Systems Manager** (faculty-equivalent permanent position), Cherry L. Emerson Center for Scientific Computation, Emory University, Atlanta, GA, U.S.A., May 1998 – April 2006.
- **Research Associate**, Department of Chemistry, Emory University, Atlanta, GA, U.S.A. April 1997 – April 1998.

CERTIFICATIONS

- IBM Certified Systems Administrator for AIX 4.3.

UNIVERSITY AND DEPARTMENTAL SERVICE

Nagoya University

- PI and/or Co-PI in Department Level Research Proposals:
  - PI, World Premier International Research Center Initiative (WPI), Institute of Transformative Bio-Molecules, 2012 – 2017.
  - Co-PI, Leading Graduate School Program (IGER), 2012 – 2017.
  - Co-PI, G30 English Undergraduate and Graduate Program, 2011 – 2017.
  - Co-PI, Global Center of Excellence (GCOE), 2006 – 2012.
  - Co-PI, CAMPUS ASIA, 2012 – 2017.
- G30 Faculty and Student Recruitment Committee
- Graduate Admissions Committee
- Department of Chemistry Faculty Recruitment Committee
- Chemistry Library Committee

CURRENT EXTERNAL FUNDING

PI Total Project Funding: USD 1.160M.

- **ORNL** Lab Directed Research and Development (LDRD) 8581, title: "*Development and Application of Computational Methodologies for the Investigation of Soft Matter Molecular and Electronic Structure and Dynamic Properties",* USD 1.160M. May 2017 – April 2019.

PAST EXTERNAL FUNDING (Currency Exchange Rates as of May 6, 2016)

PI Total Project Funding: USD 9,500, JPY 161,507K (USD 1.21M), EUR 16,000 (18K). **Total amount in USD: 1.23M.**

- **JSPS-AvH** Postdoctoral Fellowship P15778 for Dr. Kai Welke, title: *"Implementing and applying a novel strategy to enable efficient quantum-mechanical simulations of large systems",* JPY 8,216K. November 2015 – April 2017.
- Collaboration research grant from **DENSO** Corp., Nisshin, Japan entitled *"DFTB Simulation of SiC plasma synthesis"*, JPY 1,000K. April 2015 – March 2016.

- **JSPS** special research grant "KAKENHI (Kiban C)" 26410013 entitled *"Development of a direct kinetic Monte Carlo method for the investigation of nanostructure formation processes"*, JPY 4,680K. April 2014 – March 2017.
- **JSPS** World Premier Initative (WPI) – Institute of Transformative Bio-Molecules (ITbM), Nagoya University. Funding to my group includes salary for one Associate Professor, one Assistant Professor, two postdoctoral researchers, and one secretary, approximately JPY 110,000K, as well as a budget for computer equipment, approximately JPY 34,000K. January 2013 – March 2018.
- Collaboration research grant from **DENSO** Corp., Nisshin, Japan entitled *"DFTB Simulation of Carbon Materials"*, JPY 1,000K. April 2015 – March 2016.
- Bilateral **JSPS**-Australian "Open Partnership (Sakura)" Collaborative Research Project, JPY 4,785K. October 2013 – July 2015.
- Collaboration research grant from **DENSO** Corp., Nisshin, Japan entitled *"DFTB Simulation of Carbon Materials"*, JPY 1,000K. April 2014 – March 2015.
- **IAEA** Coordinated Research Project (CRP), title: *"Data for Erosion and Tritium Retention in Be",* Total Funding: EUR 16,000. January 2012 – December 2016.
- **JSPS** Postdoctoral Fellowship P12333 for Dr. Tim Kowalczyk, title: *"Development of excited state dynamics simulations to probe the photophysics of large organic molecules",* JPY 8,216K. September 2012 – March 2014.
- **JSPS** Predoctoral Fellowship PE13041 for Mr. Pablo Arturo Aparicio Sanchez, title: *"Development of a POM model redox chemical system for joint experimental and theoretical studies",* JPY 2,372K. July – November 2013.
- US-Japan Joint Institute of Fusion Theory (**JIFT**) invitation to Dr. Predrag S. Krstic to Nagoya University and Kyoto University, title: *"Quantum chemical simulation of W-C-H-He systems",* USD 4,500. February 17 – March 1, 2013.
- **JSPS-AAS** Postdoctoral Fellowship P10798 for Dr. Matt Addicoat, title: *"Elucidation of the properties and dynamic behaviour of Room Temperature Ionic Liquids (RTILs) at transition metal and graphitic surfaces using Self-Consistent Charge Density Functional Tight Binding (SCC-DFTB)",* JPY 11,888K. November 2010 – October 2012.
- **Academic Consortium 21 (AC21)** Special Project Fund with Profs. Vudhichai Parasuk (Chulalongkorn University, Bangkok, Thailand) and Supa Hannongbua (Kasetsart University, Bangkok, Thailand), entitled: *"Collaborative computational studies of cellulose degradation in ionic liquids for biofuel production",* USD 5,000. April 2011 – March 2012.
- **JSPS** Grant-in-aid "KAKENHI (Kiban C)", 20550012, entitled *"Quantum Chemical Investigation of Carbon Nanotube Functionalization and Oxidation"*, JPY 5,200K. April 2008 – March 2011.
- **JSPS** Grant-in-aid in Priority Area "Molecular Theory for Real Systems", "KAKENHI (Tokutei)", 20038023, entitled *"Quantum Chemical Investigation of Dispersion Interaction in Multilayer Carbon Onions and Nanotubes"*, JPY 2,050K. April 2008 – March 2010.
- **JSPS** special research grant "KAKENHI (Tokutei)" entitled *"Quantum Chemical Investigation of Dispersion Interaction in Multilayer Carbon Onions and Nanotubes"*, JPY 1,100K. June 2007 – March 2008.

Co-PI Total Project Funding: USD 1,193,569, JPY 506,788K (USD 474K), RUB 36,200,000 (USD 547K), EUR 723,600 (USD 827K). **Total amount in USD: 3.00M.**

- Co-PI with Prof. Alexander S. Fedorov (Kirensky Institute of Physics, Siberian Branch of Russian Academy of Science (KIP), Krasnoyarsk) as PI on a Japanese-Russian bilateral program, Russian Federal Program No.2.1 "Research and development in priority areas of scientific-technological complex of Russia in 2014–2020 years", grant number 14.613.21.0010 from the Russian Foundation for Basic Research (**RFBR**), entitled *"Development of the endohedral metallofullerenes formation theory, an efficient method of their synthesis and study of their applicability",* Total Funding: RUB 36,200,000. October 2014 – September 2020.
- Co-PI with Prof. Anastasia Vyalikh (Leibniz-Institut für Polymerforschung, Dresden) as PI on an "International Research Staff Exchange Scheme" FP7-PEOPLE-2013-IRSES, PIRSES-GA-2013-612577, European Research Council (**ERC**), Marie Curie Actions, entitled *"Tuning the properties of NanoCarbon with Fluorination",* Total Funding: EUR 207,000. October 2013 – September 2018.

- Co-PI with Prof. Thomas Heine (Jacobs University) as PI on an "International Research Staff Exchange Scheme" FP7-PEOPLE-2011-IRSES, PIRSES-GA-2011-295172, European Research Council (**ERC**), Marie Curie Actions, entitled *"Computer simulations of thermally excited molecules and materials by first principles",* Total Funding: EUR 516,600. October 2011 to September 2016.Co-PI with Prof. Shigehiro Yamaguchi (Nagoya University) as PI on a **JST**/CREST Grant entitled *"Synthesis and novel functions of soft π–materials",* Total Funding: JPY 200,000K, October 2010 – March 2016.
- Co-PI with Prof. Atsushi Ito (NIFS, Gifu) as PI on a National Institutes of Natural Sciences (**NINS**) "Young Researcher's Cross-Disciplinary Study" Program, title: *"Experimental and theoretical studies on nanomaterial formation mechanisms under nonequilibrium conditions"*, Total Funding: JPY 6,400K. April 2012 – March 2013.
- Co-PI with Prof. Keiji Morokuma as PI on a **JST**/CREST Grant entitled *"Integrated simulation of multiscale and multiphysics phenomena of complicated molecular processes"*, Total Funding: JPY 300,000K, June 2006 – March 2012.
- Co-PI with Prof. Hiroaki Nakamura on a National Institute of Fusion Science (**NIFS**) program, title: *"Quantum chemical molecular dynamics simulations of chemical hydrogen sputtering on graphite",* Total Funding: JPY 388K, April 2008 – March 2010.
- Co-PI with Prof. Kenneth K. Kuo as PI on a DoD **ONR** MURI Grant Prime Award # N00014-04-1-0683, Subaward #2794-EU-ONR-0683 entitled *"Fundamental Understanding of Propellant/Nozzle Interaction to Mitigate Erosion for Very High Pressure Missile Propellant Applications",* USD 600K, September 2004 – August 2007.
- Co-PI with Prof. Keiji Morokuma as PI on a DoD **AFOSR** DURIP Grant FA9550-04-1-0321entitled *"Workstation Cluster for Computational Studies of Chemical Reaction Systems"*, USD 213,569, May 2004 – March 2005.
- Co-PI with Prof. Keiji Morokuma as PI on an **ACS PRF** Grant 37439-AC6 entitled *"Computational Studies on Nanochemistry and Nanomaterials"*, USD 80K, January 2002 – August 2004.
- Co-PI with Prof. Keiji Morokuma as PI on an **NSF MRI** Grant CHE-0079627 for the *"Acquisition of Computer Systems for Computational Chemistry and Physics",* USD 300K, October 2000 – September 2003.

CURRENT COMPUTER TIME AWARDS

- PI on a Director Discretion Project Allocation on OLCF, Oak Ridge National Laboratory (**ORNL**) Computer Time Grant, ~**2,000,000 CPU hours** on SummitDev and Titan, February – July 2018.

PAST COMPUTER TIME AWARDS

- PI on an Institute of Molecular Science (**IMS**) Computer Time Grant, ~**200,000 CPU hours** on IMS Altix and Primequest, April 2016 – March 2017.
- PI on an Institute of Molecular Science (**IMS**) Computer Time Grant, ~**200,000 CPU hours** on IMS Altix and Primequest, April 2015 – March 2016.
- PI on an RIKEN **K Supercomputer** Time Grant, ~**20,000,000 CPU hours/year** on Fujitsu K nodes, April 2014 – March 2015.
- PI on an Institute of Molecular Science (**IMS**) Computer Time Grant, ~**200,000 CPU hours** on IMS Altix and Primequest, April 2014 – March 2015.
- PI on an Institute of Molecular Science (**IMS**) Computer Time Grant, ~**400,000 CPU hours** on IMS Altix and Primequest, April 2013 – March 2014.
- PI on an Institute of Molecular Science (**IMS**) Computer Time Grant, ~**400,000 CPU hours** on IMS Altix and Primequest, April 2012 – March 2013.
- PI on a Director Discretion Project Allocation on OLCF, Oak Ridge National Laboratory (**ORNL**) Computer Time Grant, ~**200,000 CPU hours** on Titan, June – August 2012.
- Co-PI with Dr. Jacek Jakowski as PI on an **NSF** EPSCoR TeraGrid Project entitled *"Modeling of nanoscale carbon and metalized carbon materials for the "EPSCoR Desktop to TeraGrid EcoSystems" project",* NICS, ORNL, **2,000,000 CPU hours/year** on NICS Kraken, October 2010 to July 2013.
- PI on a **NIFS** project "Quantum chemical MD simulation of graphite edge reactions with hydrogen", **1,000,000 CPU hours** on Plasma Simulator, Toki, Gifu, April 2011 – March 2012.

- PI on a **DOE** User Nanoscience Research Project CNMS2009-032 entitled *"Combined Quantum Chemical and Experimental Investigation of SWNT Growth from Metal-Decorated SWNHs"* at the Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, **unlimited access** to the ORNL Institutional Cluster (cnms.oic.ornl.gov), March 2009 – February 2011.
- Co-PI with Prof. Keiji Morokuma as PI on an Insititute of Molecular Science (**IMS**) Special Project (S) Computer Time Grant, **~900,000 CPU** hours/year on IMS Altix and Primequest, April 2007 – March 2012.
- Co-PI with Prof. Keiji Morokuma as PI on a **DOE** Grand Challenge Grant Award #GC3564 entitled *"Nanostructure Formation, Aggregation, and Reactivity",* **1,500,000 CPU hours/year** (FY06) on PNNL's MPP2 Itanium2 cluster, October 2003 – September 2009.
- PI on a **DOE** User Nanoscience Research Project CNMS2005-043 entitled *"Quantum Chemical Non-Equilibrium Dynamics of the Self-Assembly Formation Mechanisms of Fullerenes, Metallofullerenes, and Carbon Nanotubes"* at the Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, **unlimited access** to the ORNL Institutional Cluster (cnms.oic.ornl.gov), December 2005 – November 2007 plus extension 2005-043EXT until July 2008.
- Co-PI with Prof. Keiji Morokuma as PI on a **DoD** Computer Time Grant AFOSR22743227 on ARSC (Arctic Region Supercomputer Center) IBM Power4+ cluster, **~200,000 CPU hours/year**, October 2003 – September 2009 (resigned from project July 2008 due to prolonged stay in Japan).

SYNERGISTIC ACTIVITIES AND OUTREACH

1. **Member, Review Editorial Board, "Frontiers in Theoretical and Computational Chemistry"**, a section of the "Frontiers in Chemistry" Open Access journal by Swiss-based open access (OA) publisher "Frontiers in", January 2014 – present.
2. **Associate Editor, "Frontiers in Computational Materials Science"**, a section of the "Frontiers in Chemistry" Open Access journal by Swiss-based open access (OA) publisher "Frontiers in", March 2014 – September 2016.
3. **Invited member, IAEA coordinated research project (CRP)** "Erosion and Tritium Retention for Plasma Interaction with Beryllium Surfaces", IAEA, Vienna, Austria, 2012 – 2016.
4. **Organizer**, *"FMO-DFTB Mini-Workshop",* Nagoya University, Nagoya, Japan, June 20-21, 2016.
5. **Invited member, Theoretical and Computational Chemistry Initiative (TCCI)**, one of the MEXT "K supercomputer" strategic divisions of the Computational Materials Science Initiative (CMSI), project: "The Strategic Program for Innovation Research (SPIRE) Field 2, New Materials and Energy Creation", Institute for Molecular Science (IMS), Okazaki, Japan, 2010 – 2015.
6. **Member, Organization Committee**, *"NT15: Sixteenth International Conference on the Science and Application of Nanotubes",* Nagoya University, Nagoya, Japan, June 29 – July 3, 2015.
7. **Co-organizer with David Tomanek**, *"CCTN15: Tenth International Symposium on Computational Challenges and Tools for Nanotubes",* Nagoya University, Nagoya, Japan, June 28, 2015.
8. **Member, International Academic Advisory Committee**, *"The 19th International Annual Symposium on Computational Science and Engineering (ANSCSE19)",* Ubon Ratchathani, Thailand, June 17–19, 2015.
9. **Member of the International Scientific Advisory Committee**, *"7th Guadalupe Workshop on Nucleation and Growth of Single-wall Carbon Nanotubes"*, Texas, USA, April 2015.
10. **Leader, Boyscout Association of Japan**, Chapter 127, Nagoya, March 2014 – March 2015.
11. **Organizer**,*"2013 International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry (WFTCPC 2013)",* Bang Saen-Beach, Cholburi, Thailand, December 2013.
12. **Member of the International Scientific Advisory Committee**, *"International Symposium on Computational Sciences: Simulations for Material and Biological Systems",* Shanghai, China, November 2013.
13. **Organizer**, CREST-mini workshop *"Theory of Electronic Excitations in Large Molecules",* Nagoya University, Nagoya, Japan, May 29, 2013.
14. **Organizer**, *"DFTB mini-workshop",* Nagoya University, Nagoya, Japan, April 20, 2013.
15. **Member of the International Scientific Advisory Committee**, *"6th Guadalupe Workshop on Nucleation and Growth of Single-wall Carbon Nanotubes"*, Texas, USA, April 2013.
16. **Organizer**, *"FMO Workshop"* at Nagoya University by Dr. Dmitri G. Fedorov (NRI, AIST), Nagoya, Japan, March 6, 2013.

17. **International Scientific Advisory Committee Member**, *"International Symposium on Computational Sciences: Simulations for Material and Biological Systems",* Shanghai, China, August 2012.
18. **Organizer**, *"1st International Workshop on Computer Simulations of Thermally Excited Molecules and Materials by First Principles",* Nagoya University, Nagoya, Japan, March 2012.
19. Member of the Academic Consortium (AC21) Steering Committee (http://www.ac21.org), April 2011 – March 2015.
20. **Technical IAEA Advisory Committee Member** on the simulation of plasma-wall interactions, December 2011.
21. **International Scientific Advisory Committee Member**, *"International Symposium on Computational Sciences: Simulations for Material and Biological Systems",* Shanghai, China, May 2011.
22. **International Scientific Advisory Committee Member**, of the *"5th Guadalupe Workshop on Nucleation and Growth of Single-wall Carbon Nanotubes"*, Texas, USA, April 2011.
23. **Co-organizer**, *"DFTB summer school workshop"* at Kasetsart University, Nakorn Pathom, Thailand. Invited speakers were Marcus Elstner, Qiang Cui, Thomas Heine, Balint Aradi, Jacek Jakowski, Henryk Witek, Alister Page, and Stephan Irle, October 2010.
24. **Scientific Host** for 12 participants in the 2010 JENESYS (Japan-East Asia Network of Exchange for Students and Youths) program: *"Collaboratory Research and Exchange of Researchers in Simulations of Complex Molecules Using Molecular Theoretical Methods"*
25. **Scientific Host** for 9 participants in the 2009 JENESYS program: *"Collaboratory Research and Exchange of Researchers in Simulations of Complex Molecules Using Molecular Theoretical Methods"*
26. **Co-chair and organizer**, *"CREST International Symposium on Theory and Simulations of Complex Molecular Systems"*, and co-chair organizer of *"International Symposium on Theory of Molecular Structure, Function, and Reactivity, Celebrating Prof. Morokuma's 75th Birthday",* July 2009.
27. **High School Presentation,** Ichinomiya High School, Aichi Prefecture: "*Molecular dynamics simulations of inorganic molecular evolution: Self-assembly of buckminsterfullerene C_{60} and beyond",* January 2008.
28. **Co-organizer** with Dr. Djamaladdin Musaev, Emerson Center Lectureship Award Symposiums, October 2004 – April 2006)

PUBLICATIONS (see separate publication list for details)
Citation statistics (ISI Thomson Reuters): 5000+ total citations, h-factor: 38.

Peer-Reviewed Journals: 226
Book Chapters and Conference Proceedings: 31
Books edited: 2
Major Computer Codes: 2 (Contributions to COLUMBUS, GAMESS-US)

REFEREE ACTIVITIES
Research Funding Agencies
- ACS Petroleum Research Fund (ACS PRF)
- Austrian Science Funds, Austria
- Department of Energy (DOE) Basic Energy Sciences (BES), U.S.A.
- Japan Society for the Promotion of Sciences (JSPS), Japan
- National Science Foundation (NSF) EPSCoR Seed Grant program, U.S.A.
- Oak Ridge National Laboratory – Laboratory Directed Research & Development (LDRD) Program
- Research Foundation – Flanders (FWO), Belgium
- Research Grants Council, Hong Kong

Computer Time Proposals
- Panelist, Department of Energy (DOE) INCITE, U.S.A.

Scientific Journals

- ACS Applied Materials & Interfaces
- ACS Nano
- Angewandte Chemie
- Applied Catalysis A
- Bulleting of the Chemical Society of Japan
- Chemical Physics Letters
- Chemistry – A European Journal
- CNANO
- Computer Physics Communication
- Europhysics Letters
- Fullerenes, Nanotubes, and Carbon Nanostructures
- Central European Journal of Chemistry
- Chemical Science
- Chemistry Letters
- Combustion and Flame
- Computational Materials Science
- Crystal Growth & Design
- Current Organic Chemistry
- CVD Journal
- Diamond and Related Materials
- Energy & Fuels
- Environmental Science & Technology
- EPL Journal
- Inorganic Chemistry Frontiers
- International Journal of Chemical Kinetics
- International Journal of Mass Spectroscopy
- Internet Electronic Journal of Molecular Design
- Journal of Applied Physics
- Journal of the American Chemical Society
- Journal of Chemical Theory and Computation
- Journal of Computational Chemistry
- Journal of Molecular Modeling
- Journal of Molecular Liquids
- Journal of Molecular Structure (THEOCHEM)
- Journal of Nanoscience and Nanotechnology
- Journal of Nuclear Materials
- Journal of Organic Chemistry
- Journal of Organometallic Chemistry
- Journal of Physical Chemistry A/B/C
- Journal of Physics and Chemistry of Solids
- Journal of the Physical Society of Japan
- Materials & Design
- Materials Chemistry and Physics
- Materials Science & Engineering C
- Mathematical and Numerical Modeling of Flow and Transport
- Molecular Physics
- Molecular Simulation
- Nano Letters
- Nanoscale
- Nanotechnology
- Nature
- Nature Nanotechnology
- Nature Chemistry
- Philosophical Magazine & Philosophical Magazine Letters
- Physical Review A/B/Letters
- PLOS One
- RCS Advances
- Scientific Reports
- Solid State Communications
- Solid State Sciences
- Structural Chemistry
- Superlattices and Microstructures
- Theoretical Chemistry Accounts
- Zeitschrift für Physikalische Chemie

AFFILIATIONS

- American Association for the Advancement of Science, 2006 – present.
- American Chemical Society, 2003 – present.
- The Chemical Society of Japan, 2006 – present.
- Deutsche Bunsengesellschaft für Physikalische Chemie, 1992 – present.
- The Electrochemical Society, 2008 – 2016.
- The Fullerenes, Nanotubes and Graphene Research Society, 2007 –2017.
- Japan Society of Molecular Science, 2007 – 2017.
- Materials Research Society, 2012 – 2015.

PRESENTATIONS (presenter in **bold**)

International Conferences

Keynote Lectures

1. June 17–19, 2015: The 19th International Annual Symposium on Computational Science and Engineering (ANSCSE19), Ubon Ratchathani, Thailand: **S. Irle**, *"Super-reduced POM^{27-}: An Excellent Molecular Cluster Battery Component and Semipermeable Molecular Capacitor"*

2. October 4, 2014: International Symposium on "Optobiotechnology", OptoBio Technology Research Center, Nagoya Institute of Technology, Nagoya, Japan: **S. Irle,** *"On the Importance of Dynamics in Molecular Systems: From the Study of Nanostructure Formation to the Design of Photoactive Molecules"*

Invited Lectures

1. July 23–27, 2018: Workshop on "Multi-Scale Quantum Mechanical Analysis of Condensed Phase Systems: Methods and Applications", Telluride, CO, U.S.A., **S. Irle**, D. G. Fedorov, S. Ito, Y. Okamoto,*"Replica-exchange umbrella sampling in FMO-DFTB molecular dynamics: Methods and applications"*
2. August 21–25, 2017: 17th International Conference on Density-Functional Theory and its Applications, Tällberg, Sweden, **H. A. Witek,** R. Podeszwa, C.-P. Chou, Y. Nishimura, S. Irle, *"Automatized Parameterization of DFTB"*
3. November 8-11, 2016: CECAM Workshop "Approximate Quantum Methods in the *ab initio* World", Beijing Computational Science Research Center, Beijing, China: **S. Irle,** *"Replica exchange MD simulations with (linear-scaling) density-functional tight-binding"*
4. May 19–20, 2016: JCUP VII, Ohtemachi SunSky Room, Tokyo, Japan, **S. Irle,** *"Molecular dynamics investigation of the binding of auxin derivatives to auxin binding protein 1 (ABP1)"*
5. March 17–20, 2016: Computational Chemistry (CC) symposium, International Conference on Computational Methods in Science and Engineering (ICCMSE) 2016, Metropolitan Hotel, Athens, Greece, **S. Irle,** *"Molecular Dynamics in Computational Materials Sciences: From the Study of Nanostructure Formation to the Design of Fluorescent Dyes"*
6. December 15–20, 2015: Pacifichem 2015, Honolulu, HI, U.S.A.: **S. Irle**, *"A priori prediction of chemical reaction mechanisms in complex systems based on quantum chemical molecular dynamics"*.
7. December 15–20, 2015: Pacifichem 2015, Honolulu, HI, U.S.A.: **S. Irle**, *"Calculation of Charge Carrier Mobility in Covalent Organic Frameworks"*.
8. November 24–27, 2015: Molecular Designs for Advanced Materials: Workshop and Conference, Chiang Mai University, Thailand: **S. Irle**, *"Simulations of dynamic C_{60}-I_h self-assembly cut the Gordian Knot: Coexistence of bottom-up and top-down mechanisms"*.
9. June 14–17, 2015: Satellite meeting of the 15th International Congress of Quantum Chemistry: "Advances in Modeling Nano Materials", Hefei, China: **S. Irle**, *"Fun with graphenes: Quantum chemical simulations of synthesis and hydrogenation dynamics"*.
10. November 11–17, 2014: XIXth International Workshop on Quantum Systems in Chemistry, Physics and Biology (QSCP XIX), Taipei, Taiwan: **S. Irle,** H. Kitoh-Nishioka, T. Hayashi, D. Jiang, Y. Nishimoto, D. G. Fedorov, *"Calculation of Charge Carrier Mobility in Covalent Organic Frameworks"*
11. September 22–25, 2014: Fusion Conference "From Carbon-Rich Molecules to Carbon-Based Materials", El Jadida, Morocco: **S. Irle,** *"CPP fluorescence and seeded SWCNT growth mechanisms probed in quantum chemical simulations"*
12. September 13–19, 2014: Satellite Meeting "Japan-Russia Joint Symposium - Chemical Theory for Complex Systems" of the International Conference "Molecular Complexity in Modern Chemistry [MCMC-2014], Moscow, Russia: **S. Irle**, *"Recent developments for the quantum chemical investigation of systems with high structural complexity"*
13. August 17–19, 2014: 2nd CRP meeting on "Data for Erosion and Tritium Retention in Be", IAEA, Vienna, Austria: **S. Irle,** *"Progress towards accurate quantum chemical molecular dynamics simulations of plasma interactions with beryllium surfaces"*
14. August 20–22, 2014: Meeting on "Plasma-Wall Interaction with Reduced Activation Steel Surfaces", IAEA, Vienna, Austria: **S. Irle,** *"Brief review of quantum chemical calculations on H-Fe interactions"*
15. June 30–July 3, 2014: XI GIRONA SEMINAR on Carbon, Metal, and Carbon-Metal Clusters: From Theory to Applications, Girona, Spain: **S. Irle**, J. Wang, T. Kowalczyk, *"Unusual fluorescence from lanthanide-containing endohedral metallofullerenes and metal carbide fullerenes"*
16. March 10–12, 2014: Institute of Chemical Research International Symposium 2014 (ICRIS'14) "The Science and Technology of Smart Materials", Kyoto University, Uji, Japan: **S. Irle**, *"Molecular Dynamics in Computational Materials Sciences: From the Study of Nanostructure Formation to the Design of Fluorescent Dye Molecules"*

17. February 5–6, 2014: International Workshop on Atomically Controlled Fabrication Technology, Nananoshima Center, Osaka, Japan: **S. Irle**, *"Fun with graphenes: Quantum chemical simulations of synthesis and hydrogenation* dynamics"
18. December 9–13, 2013: 2013 International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry (WFTCPC'13), Bangsaen Beach, Cholburi, Thailand: **S. Irle,** *"TD-DFTB/MD Simulation of UV/Vis Fluorescence Spectra"*
19. December 9–13, 2013: 2013 International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry (WFTCPC'13), Bangsaen Beach, Cholburi, Thailand: **S. Irle,** *"Origin of the Size-Dependent Fluorescence Blueshift in [n]Cycloparaphenylenes"*
20. November 21, 2013: "International Symposium on Atomic Cluster Catalysis", Tsinghua University, Beijing, China, **S. Irle**, *"Introduction to the density-functional tight-binding (DFTB) method"*
21. November 21, 2013: "International Symposium on Atomic Cluster Catalysis", Tsinghua University, Beijing, China, **S. Irle**,*"Changes in Molecular and Electronic Structure of POM Clusters in Batteries During Charging and Discharging"*
22. November 18–20, 2013: "The Third International Symposium on Computational Sciences: Advanced Methods, Software and HPC Architectures, and Their Applications in Computational Material and Biological Sciences", Shanghai, China: M. A. Addicoat, Y. Nishimura, H. A. Witek, A. J. Page, **S. Irle**, *"Recent developments for the quantum chemical investigation of systems with high structural complexity"*
23. November 16, 2013: "International Symposium on Molecular Simulations in Biology, Chemistry, and Physics", Nagoya University, Japan, Satellite meeting of the "3rd International Conference on Molecular Simulation" in Kobe, Japan: **S. Irle**, *"Recent developments for the quantum chemical investigation of systems with high structural complexity"*
24. November 11–12, 2013: 16th IRTG Joint Symposium, Münster, German, **S. Irle**, *"Changes in Molecular and Electronic Structure of POM Clusters in Batteries During Charging and Discharging"*
25. November 11–12, 2013: 16th IRTG Joint Symposium, Münster, Germany, **Y. Nishimoto**, R. Ushimaru, T. Fujimori, D. Yokogawa, H. Naka, S. Saito, S. Irle, *"Theoretical and Experimental Mechanistic Studies of a Rh(I)-Catalyzed Aldol-type Reaction of Organonitriles Under Mild Conditions"*
26. October 21–23, 2013: Workshop "Synthesis and Spectroscopy of Large Carbon Molecules", Institute for Theoretical Atomic, Molecular, and Optical Physics (ITAMP), Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, U.S.A.: **S. Irle**, *"Molecular Dynamics Simulations of Fullerene Formation Reveal Elements of Darwinian Natural Selection"*
27. July 10–13, 2013: The Sixth Asia-Pacific Conference of Theoretical and Computational Chemistry (APCTCC 6), Gyeongju, Korea: M. A. Addicoat, Y. Nishimura, H. A. Witek, A. J. Page, **S. Irle**, *"Recent developments for the quantum chemical investigation of systems with high structural complexity"*
28. July 10–13, 2013: The Sixth Asia-Pacific Conference of Theoretical and Computational Chemistry (APCTCC 6), Gyeongju, Korea: **A. J. Page**, H.-B. Li, S. Irle, K. Morokuma, *"Control of Carbon Nanotube Chirality by Organic Templates: A Growth Mechanism from Quantum Chemical Simulations"*
29. June 14–15, 2013: International Symposium on Homogeneous Chemical Reactivity, Ibaraki University, Mito, Japan: **S. Irle**, *"Rh(I)-catalyzed Aldol-type Reaction of Organonitriles Under Mild Conditions: Theoretical Investigations"*
30. May 12–16, 2013: 223rd Electrochemical Society Meeting, Toronto, Canada, Session H3: J. Wang, T. Kowalczyk, **S. Irle**, *"Theoretical Studies of Photoluminescence Properties of Endohedral Metallofullerenes"*
31. April 12–16, 2013: The Sixth NASA – Air Force Research Laboratory – Honda – Rice University Workshop on Nucleation and Growth Mechanisms of Single Wall Carbon Nanotubes, San Antonio, Texas, USA: **S. Irle**, "*SWCNT Growth from Chiral and Achiral Carbon Nanorings: Prediction of Chirality and Diameter Influence on Local Growth Rates"*
32. January 23–25, 2013: "Pure and Applied Chemistry International Conference (PACCON) 2013", Burapha University and Chemical Society of Thailand, Bangsaen Beach, Chon Buri, Thailand: **S. Irle,** *"Origin of the Size-Dependent Fluorescence Blueshift in [n]Cycloparaphenylenes"*

33. December 1–3, 2012: 2012 International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry (WFTCPC'12), Hong Kong Baptist University, Hong Kong: **S. Irle,** *"Origin of the Size-Dependent Fluorescence Blueshift in [n]Cycloparaphenylenes"*

34. September 26 – 28, 2012: 1st CRP meeting on "Data for Erosion and Tritium Retention in Be", IAEA, Vienna, Austria: **S. Irle,** *"Towards accurate approximate density functional theory potentials for beryllium-plasma interactions"*

35. August 12–15, 2012: "International Symposium on Computational Sciences: Simulations for Material and Biological Systems", Shanghai, China: **S. Irle**, *"Quantum Chemical MD Simulations of Graphene Formation"*

36. May 10–12, 2012: "JST International Symposium on Multi-Scale Simulation of Condensed-Phase Reaction Systems", Nagoya University, Japan: **S. Irle**,*"Autocatalytic networks of chemical reaction processes in high-temperature materials science"*

37. May 6–11, 2012: 221st Electrochemical Society Meeting, Seattle, WA, U.S.A.: D. Kazachkin, Y. Nishimura, H. A. Witek, S. Irle, **E. Borguet**, *"Dramatic Reduction of IR Vibrational Cross-sections of Molecules Encapsulated in Carbon Nanotubes"*

38. April 9–13, 2012: 2012 Materials Research Society Spring Meeting, San Francisco, CA, U.S.A.: K. Usui, Y. Nishimoto, A. J. Page, H. A. Witek, **S. Irle**, *"The molecular structure and vibrational spectroscopy of hydroxylated nanodiamonds"*

39. March 12–13, 2012: "1st Campus Asia Symposium", Nagoya University, Japan: **S. Irle**, *"Quantum Chemistry of Complex Systems"*

40. March 10–11, 2012: 1st International Workshop on Computational Simulations of Thermally Excited Molecules and Materials by First Principles, Nagoya University, Nagoya, Japan: **J. Jakowski,** S. Irle, K. Morokuma, *"Electron and energy transfer in carbon materials from quantum dynamics simulations"*

41. December 14–15, 2011: Technical Meeting on "Ab-Initio Based Methods for Plasma-Material Interaction in Fusion Devices", IAEA, Vienna, Austria: **S. Irle,** *"Density-Functional Tight-Binding Molecular Dynamics for Chemical Sputtering Simulations"*

42. December 9–11, 2011: International Symposium on EcoTopia Science (ISETS) 2011, Nagoya University, Nagoya, Japan: **S. Irle**, *"Atomistic mechanism of graphene formation as predicted by nonequilibrium quantum chemical molecular dynamics simulations"*

43. October 3–4, 2011: IRTG Meeting, Nagoya University, Nagoya, Japan, **S. Irle,** *"Origin of the unusual blue-shift of [n]cycloparaphenylene fluorescence with increasing size n"*

44. July 17–22, 2011: Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists, Santiago de Compostella, Spain, Y. Wang, **S. Irle**, *"QM/MD Simulation of Graphene Hydrogenation"*

45. April 30–May 6, 2011: 219th Electrochemical Society Meeting, Montreal, Canada, Session H5: J. Wang, **S. Irle**, *"Erbium Photoluminescence in $Er_2C_2@C_{82}$ and $Er_2@C_{82}$ Elucidated by Density Functional Theory"*

46. April 30–May 6, 2011: 219th Electrochemical Society Meeting, Montreal, Canada, Session H6: Y. Nishimoto, Benjamin Finck, Z. Wang, Keiji Morokuma, **S. Irle**, *"New Insights from Quantum Chemical Molecular Dynamics Simulations on the Formation Mechanism of Metallofullerenes"*

47. April 18–21, 2011: International Symposium on Computational Sciences: Quantum Simulations for Material and Biological Systems", Shanghai, China: **S. Irle**, "*QM/MD Simulations of Graphene Hydrogenation"*

48. April 8–12, 2011: The Fifth NASA – Air Force Research Laboratory and Rice University Workshop on Nucleation and Growth Mechanisms of Single Wall Carbon Nanotubes, San Antonio, Texas, USA: **S. Irle**, "*Accurate atomic-scale molecular dynamics simulations of SWCNT nucleation, growth, and healing"*

49. October 14, 2010: DFTB summer school workshop at Kasetsart University, Bangkok, Thailand: **S. Irle**, *"Quantum chemical molecular dynamics simulations of combustion fullerene synthesis",*

50. October 14, 2010: DFTB summer school workshop at Kasetsart University, Bangkok, Thailand: **A. J. Page**, S. Irle, and K. Morokuma, *"Simulation of Nanoscale Self-Assembly Processes using Density-Functional Tight-Binding Molecular Dynamics"*

51. September 20–24, 2010: CeCAM meeting on Approximate Quantum-Methods: Advances, Challenges & Perspectives, Bremen, Germany, **S. Irle**, *"Application of the DFTB Method to Nano Structure Dynamics and to ONIOM(QM:QM) and ONIOM(QM:QM:MM) Methods"*

52. July 19–21, 2009: Nano Session, CREST International Symposium on Theory and Simulations of Complex Molecular Systems, Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, Japan: **S. Irle**, K. Morokuma, *"Density-functional tight-binding molecular dynamics simulations of carbon nanotube formation"*.
53. May 24–29, 2009: 215th Electrochemical Society Meeting, San Francisco, CA, U.S.A., Session H5: **S. Irle**, *"Quantum chemical molecular dynamics simulations of giant metallofullerene formation"*
54. May 24–29, 2009: 215th Electrochemical Society Meeting, San Francisco, CA, U.S.A., Session H6: **S. Irle**, *"On the Driving Force for Irreversible C_2 Elimination from Giant Fullerenes at High Temperature"*
55. December 9–13, 2008: IUMRS-ICA 2008, Nagoya Congress Center, Nagoya, Japan: **S. Irle**, *"Continued Growth of Single-Walled Carbon Nanotubes on Iron Catalyst Particles in Density-Functional Tight-Binding Molecular Dynamics*"
56. September 14–19, 2008: WATOC 2008, Sydney, Australia, Y. Ohta, Y. Okamoto, S. Irle, **K. Morokuma**, *"Growth Process of Single-Walled Carbon Nanotubes from Metal Cluster: Density Functional Tight-Binding Molecular Dynamics Simulation"*
57. May 18–23, 2008: 213th Electrochemical Society Meeting, Electron Transfer and Applications of Fullerene and Nanostructured Materials, in Honor of David Schuster, Phoenix, Arizona, U.S.A., **S. Irle**, *"Quantum Chemical Molecular Dynamics Simulations of Dynamic Fullerene and Carbon Nanotube Self-Assembly"*.
58. August 2007: 234th ACS National Meeting, Boston, Massachusetts, U.S.A.: **K. Morokuma**, S. Irle, Z. Wang, G. Zheng, B. Finck, B. Saha, Y. Ohta, and Y. Okamoto, *"Quantum Chemical Molecular Dynamics Simulations of Growth of Fullerenes, Metallofullerenes, and Carbon Nanotubes"*
59. September 2006: 232nd ACS National Meeting, San Francisco, California, U.S.A.: **S. Irle**, *"DFTB-based QM/MD simulations of nanostructure formation processes far from thermodynamic equilibrium"*.

Contributed Talks

1. March 18-22, 2018: 255th ACS National Meeting, New Orleans, LA, U.S.A.: **H. Kitoh-Nishioka**, K. Welke, Y. Nishimoto, D. G. Fedorov, S. Irle, *"Multiscale Simulations on Charge Transport in Covalent Organic Frameworks"*; **Q. V. Vuong**, J. Kuriappan, M. Kubillus, J. Kranz, T. Mast, T. Niehaus, S. Irle, M. Elstner, *"Parametrization and benchmark of the range separated LC-DFTB2 method for organic molecules"*; **K.-H. Lee**, U. Schnupf, S. Irle, *"Theoretical investigations of simple carbohydrates by density-functional tight-binding: A comparative analysis to density"*
2. March 18-22, 2018: 255th ACS National Meeting, New Orleans, LA
3. March 18-22, 2018: 255th ACS National Meeting, New Orleans, LA
4. February 18-23, 2018: The 58th Sanibel Symposium, St. Simons Island, GA, U.S.A.: **H. Kitoh-Nishioka**, K. Welke, Y. Nishimoto, D. G. Fedorov, S. Irle, *"Multiscale Simulations on Charge Transport in Covalent Organic Frameworks"*
5. September 16–17, 2013: 2013 JSAP-MRS Joint Symposium "High-Performance Computing and Electronic Structure Calculations in Materials Research", Kyoto, Japan: **S. Irle**, *"Quantum chemical MD simulations of chirality-controlled carbon nanotube growth and edge-controlled graphene nanoribbon synthesis"*

6. May 12–16, 2013: 223rd Electrochemical Society Meeting, Toronto, Canada, Session H4: Y. Nishimura, H. A. Witek, **S. Irle**, *"First Principles-Based Estimate of the Critical SWCNT Length for Raman D and G Band Intensity Inversion"*

7. May 9–11, 2013: 112th Bunsentagung (Annual German Conference on Physical Chemistry), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany: **S. Irle,** C. Camacho, Th. Niehaus, *"Temperature effect of the fluorescence blueshift in [n]cycloparaphenylenes with increasing molecular size"*
8. April 18–19, 2013: The 1st International Symposium on Transformative Bio-Molecules 2013, Nagoya University, Nagoya, Japan: **S. Irle**, *"Quantum Chemistry of Complex Systems"*
9. August 19 – 23, 2012: 244th ACS National Meeting, Philadelphia, PA, U.S.A., **J. Jakowski,** S. Irle, K. Morokuma, *"Collision of neutral and charged fullerenes as a prototype of non-equilibrium, non-adiabatic redox reaction – quantum dynamics simulations"*
10. April 9–13, 2012: 2012 Materials Research Society Spring Meeting, San Francisco, CA, U.S.A.: Y. Wang, A. J. Page, Y. Nishimoto, H.-J. Qian, K. Morokuma, **S. Irle**, *"Haeckelite and Graphene Formation on a Metal Surface: Evidence for a Phase Transformation at the Edge of Criticality"*

11. March 10–11, 2012: 1st International Workshop on Computational Simulations of Thermally Excited Molecules and Materials by First Principles, Nagoya University, Nagoya, Japan: **C. Camacho**, S. Irle, *"The temperature effect in the fluorescence blueshift in [n]cycloparaphenylenes with increasing molecular size"*
12. March 10–11, 2012: 1st International Workshop on Computational Simulations of Thermally Excited Molecules and Materials by First Principles, Nagoya University, Nagoya, Japan: **A. J. Page**, Y. Wang, H.-B. Li, S. Irle, K. Morokuma, *"Carbon Nano-Structure Self-Assembly: Insights from QM/MD Simulations"*
13. December 9–13, 2011, The Fifth Asian Pacific Conference of Theoretical & Computational Chemistry, Rotorua, New Zealand, **M. Addicoat,** S. Irle, *"CrazyLego: Building ionic liquid clusters block by block"*
14. September 11–17, 2011, QSCP-XVI, Kanazwa, Japan: **H. Kono,** N. Niitsu, K. Yamazaki, K. Nakai, M. Toda, S. Irle, *"Control of Vibrational Dynamics and Reaction of C_{60} and Its Derivatives by Near-Infrared Fields"*
15. September 11–17, 2011, QSCP-XVI, Kanazwa, Japan: S. Irle, A. J. Page, B. Saha, Y. Wang, K. R. S. Chandrakumar, Y. Nishimoto, H.-J. Qian, **K. Morokuma**, *"Nucleation, Growth and Healing Processes of Single-Walled Carbon Nanotubes from Metal Clusters and SiO_2 and SiC Surfaces: Density Functional Tight-Binding Molecular Dynamics Simulation"*
16. September 2–8, 2011: The 7th Congress of the International Society for Theoretical Chemical Physics (ISTCP), Waseda University, Tokyo, Japan: **M. Addicoat**, A. J. Page, Z. Brain, L. Flack, K. Morokuma, S. Irle, *"An Optimized Genetic Algorithm for the Functionalization of Fullerenes"*
17. September 2–8, 2011: The 7th Congress of the International Society for Theoretical Chemical Physics (ISTCP), Waseda University, Tokyo, Japan: **A. J. Page,** Y. Wang, KRS Chandrakumar, S. Irle, K. Morokuma, *"Mechanisms of Carbon-Based Nanostructure Self-Assembly: Insights from Density-Fuctional Tight-Binding Molecular Dynamics"*
18. September 2–8, 2011: The 7th Congress of the International Society for Theoretical Chemical Physics (ISTCP), Waseda University, Tokyo, Japan: **S. Irle**, Y. Nishimoto, B. Finck, Z. Wang, K. Morokuma, *"New Insights from Quantum Chemical Molecular Dynamics Simulations on the Formation Mechanism of Metallofullerenes"*
19. July 24–29, 2011: Carbon 2011, Shanghai, China: **H.-J. Qian**, Y. Wang, K. Morokuma, S. Irle, *"QMMM/MD Simulations of Dynamics Small Fullerene Formation in Carbon Vapor With Inert Carrier Gas"*
20. July 17–22, 2011: Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists, Santiago de Compostella, Spain: **A. J. Page**, KRS Chandrakumar, S. Irle, K. Morokuma, *"Understanding Nanoscale Self-Assembly Processes Using QM/MD: Mechanisms of Carbon Nanotube Nucleation and Growth"*
21. April 18–21, 2011: International Symposium on Computational Sciences: Quantum Simulations for Material and Biological Systems", Shanghai, China: **Y. Wang,** H.-J. Qian, Y. Ohta, K. Morokuma, S. Irle, "*QM/MD Simulations of CNT Nucleation on Iron Nanoparticles Using Acetylene Feedstock"*
22. February 26 – March 5, 2011: 25th International Winterschool on Electronic Properties of Novel Materials, Kirchberg, Austria, **D. Haberer**, D. Usachov, C. Giusca, M. Farjam, S. A. Jafari, S. Taioli, Y. Wang, B. Dora, H. Sachdev, T. Pichler, S. R. P. Silva, S. Irle, M. Knupfer, B. Büchner, A. Grüneis, *"Electronic Properties of Functionalized Quasi-Free-Standing Graphene and Monolayer Boron Nitride"*
23. December 15–20, 2010: Pacifichem 2010, Honolulu, HI, U.S.A.: Y. Nishimura and **S. Irle**, *"Quantum chemical investigations of small molecules on graphitic systems: energetics, dynamics, and vibrational spectropscopy"*
24. December 15–20, 2010: Pacifichem 2010, Honolulu, HI, U.S.A.: A. Page, Y. Ohta, Y. Okamoto, Y. Wang, M. Soma, **S. Irle,** and K. Morokuma, *"Mechanisms for Single-Walled Carbon Nanotube Nucleation, Growth, and Healing Determined Using Quantum Chemical Molecular Dynamics Methods"*
25. July 11–17, 2010: Carbon 2010, Clemson University, SC, U.S.A.: **Y. Wang,** Y. Ohta, H.-J. Qian, K. Morokuma, and S. Irle, *"Early Stages in the Nucleation Process of Carbon Nanotubes: Density-Functional Tight-Binding Molecular Dynamics Simulations of Acetylene Polymerization and Cross-Linking on an Fe38 Particle"*

26. June 27, 2010: CCNT10 – Sixth International Symposium on Computational Challenges and Tools for Nanotubes, Hilton Bonaventure, Montreal, Canada: **Y. Wang**, Y. Ohta, H.-J. Qian, K. Morokuma, and S. Irle, *"Early Stages in the Nucleation Process of Carbon Nanotubes: Density-Functional Tight-Binding Molecular Dynamics Simulations of Acetylene Polymerization and Cross-Linking on an Fe38 Particle"*
27. May 25, 2010: The 9th joint seminar of IRTG program, Nagoya University, Japan: **L. Liu** and S. Irle, *"Migration behavior of graphene vacancy defects at elevated temperatures"*
28. June 20, 2009: CCNT09 - Fifth International Symposium on Computational Challenges and Tools for Nanotubes, Tsinghua University, Beijing, China, **A. J. Page**, Y. Ohta, Y. Okamoto, S. Irle, K. Morokuma. *"Zigzag Grows Faster Than Armchair: Comparisons of SWNT Growth From Self-Consistent-Charge Density-Functional Tight-Binding Molecular Dynamics Simulations."*
29. March 22–30, 2009: 237th ACS National Meeting, Salt Lake City, Utah, U.S.A., **S. Irle**, *"*Ab initio *and DFT studies of atomic hydrogen chemisorption on model graphite compounds".*
30. February 24–March 2, 2010: Sanibel Symposium, St. Simons Island, GA, U.S.A., A. J. Page, S. Irle, Y. Ohta, Y. Okamoto, G. Zheng, Z. Wang, Y. Wang, and **K. Morokuma**, *"Nucleation, Growth, and Healing Processes of Single-Walled Carbon Nanotubes form Metal Cluster: Density-Functional Tight-Binding Molecular Dynamics Studies"*
31. December 2007: 2nd Japan-Czech-Slovakia Joint Symposium for Theoretical/Computational Chemistry, Kyoto University, Japan: **B. Saha**, S. Irle K. Morokuma, *"Quantum chemical molecular dynamics simulations of polycyclic aromatic hydrcarbon formation during benzene combustion"*
32. August 18–25, 2007: 234th ACS National Meeting, Boston, Massachusetts, U.S.A., **S. Irle**, *"Entrapment of Metals and C_2 Inside Fullerenes On the Shrinking Hot Giant Road: Quantum Chemical Molecular Dynamics Simulations".*
33. August 18–25, 2007: 234th ACS National Meeting, Boston, Massachusetts, U.S.A.**, Z. Wang,** S. Irle, K. Morokuma, *"Graphene growth during sublimation decomposition of SiC: A quantum chemical molecular dynamics investigation"*
34. August 18–25, 2007: 234th ACS National Meeting, Boston, Massachusetts, U.S.A., **S. Irle**, *"Quantum Chemical Molecular Dynamics Simulations of Carbon Nanotube Self-Assembly on Transition Metal Catalysts".*
35. September 2006: 232nd ACS National Meeting, San Francisco, California, U.S.A., **S. Irle**, *"The Use of ONIOM in Computational Nanomaterials Research".*
36. September 2006: 232nd ACS National Fall Meeting, San Francisco, California, U.S.A., S. Irle, G. Zheng, Z. Wang, and **K. Morokuma**, *"QM/MD simulations of carbon nanotube and fullerene growth and dynamics"*
37. September 2006: 232nd ACS National Fall Meeting, San Francisco, California, U.S.A.**, Talk**: **Z. Wang**, S. Irle, G. Zheng, and K. Morokuma, *"Quantum chemical molecular dynamics study of catalyst-free SWNT growth from SiC-derived carbon"*
38. March 2006: 231th ACS National Meeting, Atlanta, Georgia, U.S.A., **S. Irle**, *"High-T Quantum Chemical Molecular Dynamics and Experiment Agree: SWNT Caps Grow Catalyst-Free with Chirality Preference on SiC Surfaces"*
39. March 2005: 229th ACS National Spring Meeting, San Diego, California, U.S.A., **Talk**: **A. A. Viggiano**, A. Midey, P. Zhang, S. Irle, K. Morokuma, *"Ion chemistry important for the ionosphere and atmospheric discharges: Kinetics of nitrogen and oxygen containing species at high temperatures"*
40. March 2005: 229th ACS National Spring Meeting, San Diego, California, U.S.A., **Talk**: S. Irle, G. Zheng, H. A. Witek, **K. Morokuma**, and M. Elstner, *"Density functional tight binding (DFTB) method and its application to molecular dynamics simulations of formation of fullerenes and carbon nanotubes"*

Domestic Conferences

Invited Talks

3. January 10–11, 2014: Supercomputer Workshop 2014, Okazaki Conference Hall, Okazaki, Japan: **S. Irle,** *"Game-Changing Influence of Excited States Dynamics for Photoemission Properties of π−Conjugated Molecular Dyes"*

4. November 5–6, 2013: TCCI 3rd Symposium for Communicating with Experimental Chemists, Fukui Institute of Fundamental Chemistry, Kyoto University, Kyoto, Japan: **S. Irle,** *"Changes in Molecular and Electronic Structure of Metal Oxide Clusters in Batteries During Charging and Discharging"*
5. February 10–11, 2012: NINS Symposium "Hierarchy Structure in Nature Revealed by Simulation", Abo Hall, Nagoya, Japan: **S. Irle,** *"Principles of Darwinian Evolution Revealed in Quantum Chemical MD Simulations of Graphene Synthesis and Hydrogenation"*
6. September 22, 2011: Physical Society of Japan Autumn Meeting, Toyama, **W. Norimatsu**, M. Morita, M. Kusunoki, and S. Irle, *"Molecular dynamics simulation of graphene formation on SiC(0001)"*
7. September 13, 2010: Symposium on Global Reaction Route Mapping (GRRM), Fukui Institute for Fundamental Chemistry, Kyoto University, **S. Irle,** *"Holes in graphite and how to repair them"*
8. September 1–4, 2010: GCOE meeting of the Department of Chemistry, Tohoku University, Sendai: *"Graphene: molecular structure, vibrational spectroscopy, and hydrogen chemisorption"*
9. August 9, 2010: IMS Okazaki: **S. Irle,** *"Current state and future directions of quantum chemical MD simulations"*
10. July 9, 2010: IMS Okazaki: **S. Irle,** *"Bears, Bubbles, and Hot Carbon"*
11. October 3–4, 2008: 2008, Hazu Onsen: **S. Irle,** *"Recent progress in quantum chemical molecular dynamics simulations of giant metallofullerene formation"*
12. February 2007: The 32nd F-NT Symposium at Meijo University, Nagoya, Japan: **S. Irle,** *"Quantum Chemical Molecular Dynamics Simulations of Fullerene and Carbon Nanotube Self-Assembly"*

Contributed Talks

1. September 3–5, 2014: 47th Fullerene-Nanotubes-Graphene General Symposium, Nagoya University, Nagoya: **S. Irle**, *"Simulations of dynamic C_{60}-I_h self-assembly cut the Gordian Knot: Coexistence of bottom-up and top-down mechanisms"*
2. May 22–24, 2014: The 17th Annual Meeting of Theoretical Chemistry, Nagoya University, Nagoya, Japan: **K. Usui**, D. Yokogawa, S. Irle, *"Theoretical Studies of Two-Photon Absorption Properties of Molecules with a Stilbene Framework"*
3. March 22–25, 2014: The 94th Annual Spring Meeting, Chemical Society of Japan, Nagoya University, Nagoya, Japan: **C. Mori,** S. Saito, C. Yuan, C. Camacho, S. Irle, S. Yamaguchi, *"Environment-Dependent Multiluminescence of a Flexible Acene Derivative"*
4. March 22–25, 2014: The 94th Annual Spring Meeting, Chemical Society of Japan, Nagoya University, Nagoya, Japan: **Y. Nishimoto,** D. Yokogawa, H. Yoshikawa, K. Awaga, S. Irle, *"Formation of Metal Atom Triangles Accompanies the Super-Reduction of Polyoxometalate (POM) Clusters"*
5. March 22–25, 2014: The 94th Annual Spring Meeting, Chemical Society of Japan, Nagoya University, Nagoya, Japan: **Y. Nishimoto,** D. Yokogawa, H. Yoshikawa, K. Awaga, S. Irle, *"Formation of Metal Atom Triangles Accompanies the Super-Reduction of Polyoxometalate (POM) Clusters"*
6. October 8–11, 2013: 36th Symposium on Solution Chemistry of Japan, Hokkaido, Japan: **K. Usui**, D. Yokogawa, S. Irle,*"Theoretical study of the charge transfer process in the fluorescent probe using RISM-SCF-SEDD"*
7. September 24–27, 2013: Annual Meeting of Japan Society for Molecular Science, Kyoto, Japan: **Arifin**, D. Yokogawa, S. Irle, *"Theoretical Study of Glucose Hydrolysis Mechanisms using RISM-SCF-SEDD"*
8. March 26–28, 2013: "2013 Workshop on 3DRISM/RISM: Present and Future", Ritsumeikan University, Shiga Prefecture, Japan: **Arifin**, D. Yokogawa, S. Irle,*"Quantum chemical study of glucose hydrolysis in acidic environment using RISM-SCF-SEDD"*
9. March 26–28, 2013: "2013 Workshop on 3DRISM/RISM: Present and Future", Ritsumeikan University, Shiga Prefecture, Japan: **K. Usui**, D. Yokogawa, S. Irle,*"Theoretical Study of Electron Transfer in Water"*
10. March 22–25, 2013: The 93rd Annual Spring Meeting, Chemical Society of Japan, Ritsumeikan University, Shiga Prefecture, Japan: **S. Irle**, Y. Nishimura, A. S. Fedorov, H. A. Witek, *"Kinetic Stability Governs Relative Fullerene Isomer Abundance"*
11. March 22–25, 2013: The 93rd Annual Spring Meeting, Chemical Society of Japan, Ritsumeikan University, Shiga Prefecture, Japan: **E. Yamaguchi**, A. Fukazawa, A. Feldmann, Y. Kousaka, K. Usui, D. Yokogawa, S. Irle, G. Erker, S. Yamaguchi, *"Fluorescence and Excited State Dynamics of π-Extended Phosphole Oxides at 3 Position"*

12. March 22–25, 2013: The 93rd Annual Spring Meeting, Chemical Society of Japan, Ritsumeikan University, Shiga Prefecture, Japan: **S. Saito**, C. Yuan, C. Camacho, T. Kowalczyk, S. Irle, S. Yamaguchi, *"RGB triple-color emissions from a single luminophore"*

13. March 22–25, 2013: The 93rd Annual Spring Meeting, Chemical Society of Japan, Ritsumeikan University, Shiga Prefecture, Japan: **K. Usui**, D. Yokogawa, S. Irle, *"Theoretical Study of Electron Transfer in a Liquid Medium"*

14. March 22–25, 2013: The 93rd Annual Spring Meeting, Chemical Society of Japan, Ritsumeikan University, Shiga Prefecture, Japan: **D. Yokogawa**, S. Irle, *"Development of TD-DFT calculation coupled with RISM-SCF-SEDD and application to excited state calculation in solution"*

15. March 22–25, 2013: The 93rd Annual Spring Meeting, Chemical Society of Japan, Ritsumeikan University, Shiga Prefecture, Japan: **Y. Nishimoto**, T. Fujimori, D. Yokogawa, S. Irle, *"Theoretical Investigation of an Aldol-Type Reaction with Rh complex"*

16. March 11–13, 2013: 44th Fullerene-Nanotubes-Graphene General Symposium, The University of Tokyo, Tokyo, Japan: **S. Irle**, Y. Nishimura, A. S. Fedorov, H. A. Witek, *"Kinetic Stability Governs Relative Fullerene Isomer Abundance"*

17. March 11–13, 2013: 44th Fullerene-Nanotubes-Graphene General Symposium, The University of Tokyo, Tokyo: **Y. Nishimura**, H. A. Witek, S. Irle, *"First Principles-Based Estimate of the Critical SWCNT Length for Raman D and G Band Intensity Inversion"*

18. March 11–13, 2013: 44th Fullerene-Nanotubes-Graphene General Symposium, The University of Tokyo, Tokyo: **Y. Sado**, S. Aoyagi, N. Izumi, R. Kitaura, T. Kowalczyk, J. Wang, S. Irle, E. Nishibori, K. Sugimoto, H. Shinohara, *"Structure of Thulium and Carbon Cluster Encapsulated in Low-Symmetry $C_{82}(C_s(6))$ Fullerene Cage by Single Crystal X-ray Diffraction"*

19. December 7–8, 2012: 3rd Japanese Symposium on Ionic Liquids, Naha, Japan: **D. Yokogawa**, Y. Nishimoto, S. Irle, *"Theoretical Study of the Hydrolysis of Cellobiose to Glucose in Ionic Liquid"*

20. November 12–14, 2012: 35th Symposium on Solution Chemistry of Japan, Waseda University, Tokyo, Japan: **T. Kubota**, H. Nishizawa, H. Nakai, Stephan Irle, *"Theoretical study of carbon capture and storage (CCS) technology with DFTB-MD method"*

21. May 17–19, 2012: SETCA meeting, University of Georgia, Athens, GA, U.S.A.: **J. Jakowski,** S. Irle, B. G. Sumpter, K. Morokuma, *"Real time simulations of electron transfer and energy transfer in carbon materials"*

22. March 25–28, 2012: The 92nd Annual Spring Meeting, Chemical Society of Japan, Keio University, Yokohama, Japan: **S. Irle**, Y. Okita, L. Liu, H. Hara, *"Holes in Graphene and How to Fill Them"*

23. March 25–28, 2012: The 92nd Annual Spring Meeting, Chemical Society of Japan, Keio University, Yokohama, Japan: **S. Jin**, M. Supur, M. Addicoat, E.-M. El-khouly, X. Ding, X. Feng, A. Nagai, S. Irle, S. Fukuzumi, D. Jiang, *"Synthesis of Two-dimensional Donor Acceptor Polymers and Covalent Organic Frameworks for Photoinduced Electron Transfer and Charge Separation"*

24. March 25–28, 2012: The 92nd Annual Spring Meeting, Chemical Society of Japan, Keio University, Yokohama, Japan: **X. Chen**, Z. Guo, X. Feng, O. Saengsawang, L. Liu, A. Nagai, S. Irle, D. Jiang, *"Synthesis and Functions of Two-dimensional Conjugated Polymers"*

25. March 25–28, 2012: The 92nd Annual Spring Meeting, Chemical Society of Japan, Keio University, Yokohama, Japan: **T. Kushida**, Z. Zhou, T. Katayama, S. Ito, H. Miyasaka, E. Sakuda, N. Kitamura, S. Irle, A. Wakamiya, S. Yamaguchi, *"Photophysical Properties of Planarized Triphenylboranes"*

26. March 19–20, 2012: 2nd meeting on the "NINS development project for young researchers", Tottori University, Tottori: **S. Irle,** *"Density-Functional Tight-Binding Molecular Dynamics for Chemical Sputtering Simulations"*

27. March 1–2, 2012: "Japan-US Fusion Technology Report Meeting", Tokyo Garden Palace Hotel, Tokyo, Japan: **S. Irle,** *"Quantum Chemical MD Simulations of the Li-C-H-O System"*

28. January 30–31, 2012: "2nd CMSI Research Meeting: Towards New Materials and Energy Generation", IMR, Tohoku University, Sendai, Japan: **S. Irle,** *"pQMMD: Parallel Quantum Chemical Molecular Dynamics Simulations for the* A Priori *Prediction of Chemical Reaction Mechanisms in Complex Systems"*

29. September 29–30, 2011: "NINS Program for Cross-Disciplinary Study and NIFS collaborative research on PWI" meeting, NIFS, Toki, Gifu, Japan: Y. Wang, H.-J. Qian, **S. Irle**, A. M. Ito, H. Nakamura, D. Haberer, A. Grüneis, *"Quantum chemical molecular dynamics simulations of graphene hydrogenation"*

30. September 22, 2011: 5th Annual Meeting of Japan Society for Molecular Science (2011), Sapporo, Japan, **S. Irle,** Y. Wang, Y. Nishimoto, H.-J. Qian, A. J. Page, K. Morokuma, *"Haeckelite and graphene formation on a metal surface: Evidence for a phase transition at the edge of criticality"*
31. March 8–10, 2011: 40th Fullerene-Nanotubes General Symposium, Meijo University, Nagoya, **S. Irle**, A. J. Page, H. Yamane, Y. Ohta, K. Morokuma, *"QM/MD Simulation of SWNT Nucleation on Transition-Metal Carbide Nanoparticles"*
32. September 14–17, 2010: The 4th Annual Meeting of Japan Society for Molecular Science, Osaka University, Osaka: **Y. Nishimura,** S. Irle, *"Benchmark studies for ionic liquids adsorbed on graphitic surfaces"*
33. September 5–9, 2010: 39th Fullerene-Nanotubes General Symposium, Kyoto University, Kyoto: **K. R. S. Chandrakumar**, S. Irle, K. Morokuma, *"Growth of Nanotubes/Nanocapsules from Metal Decorated Carbon Nanocone Aggregates: Insights from DFTB-MD Simulations"*
34. September 5–9, 2010: 39th Fullerene-Nanotubes General Symposium, Kyoto University, Kyoto: **A. J. Page,** S. Irle, K. Morokuma, *"QM/MD investigation of SWNT Nucleation on SiO_2 via CH_4 CVD"*
35. June 21, 2010: 8th FIFC Seminar, Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto: **A. J. Page**, S. Irle, and K. Morokuma, *"Carbon Nanotube Nucleation on Traditional and Non-Traditional Catalysts: Insights from QM/MD Simulations"*
36. May 23–25, 2010: 13th Theoretical Chemistry Meeting, Sapporo University, Sapporo: **Y. Wang**, Y. Ohta, H.-J. Qian, K. Morokuma and K. Morokuma, *"Early Stages in the Nucleation Process of Carbon Nantoubes: Density-Functional Tight-Binding Molecular Dynamics Simulations of Acetylene Polymerization and Cross-Linking on an Fe_{38} Particle"*
37. May 23–25, 2010: 13th Theoretical Chemistry Meeting, Sapporo University, Sapporo: **J. Wang** and S. Irle, *"Molecular and Electronic Properties of Tm-containing Metallofullerenes"*
38. May 21–22, 2010: SETCA meeting, University of South Carolina, Columbia, SC, U.S.A.: **J. Jakowski**, S. Irle, K. Morokuma, *"Quantum chemical simulation of electrons on GPU: Liouville-von Neumann dynamics"*
39. March 26–29, 2010: The 90th Annual Spring Meeting, Chemical Society of Japan, Kinki University, Osaka: **L. Liu,** F. J. Martín-Martínez, J. A. Dobado, S. Irle, *"Density-Functional Tight-Binding Studies of Clar Patterns in Hexagonal Graphene Flakes and Convergence to Graphite"*
40. March 26–29, 2010: The 90th Annual Spring Meeting, Chemical Society of Japan, Kinki University, Osaka: **Y. Nishimura,** S. Irle, *"Stealth Effect in Infrared Vibrational Spectroscopy of Molecules Adsorbed on Single-Walled Carbon Nanotubes"*
41. March 26–29, 2010: The 90th Annual Spring Meeting, Chemical Society of Japan, Kinki University, Osaka: **Y. Wang**, Y. Ohta, H.-J. Qian, K. Morokuma and K. Morokuma, *"Early Stages in the Nucleation Process of Carbon Nantoubes: Density-Functional Tight-Binding Molecular Dynamics Simulations of Acetylene Polymerization and Cross-Linking on an Fe38 Particle"*
42. March 26–29, 2010: The 90th Annual Spring Meeting, Chemical Society of Japan, Kinki University, Osaka: **J. Wang** and S. Irle, *"Nature of chemical bonding in endohedral di-metallofullerenes and their carbides: $M_2(C_2)@C_{2n}$ (M=Y, La, Er, Lu, 2n=82 and 80)",*
43. March 26–29, 2010: The 90th Annual Spring Meeting, Chemical Society of Japan, Kinki University, Osaka: **H. Hara**, G. Ichinose, S. Irle, *"DFTB/MD simulations of high-temperature annealing of open-ended (n,n) SWNTs for n=3 to 10"*
44. March 6, 2010: JSPS Priority Area "Molecular Theory for Real Systems", Results Meeting, Tokyo University Komaba Campus, Japan: *"Quantum chemical investigations of small molecules on graphitic systems: Energetics, dynamics and vibrational spectroscopy"*
45. March 2–4, 2010: 38th Fullerene-Nanotubes General Symposium, Meijo University, Nagoya, **Y. Wang**, Y. Ohta, H.-J. Qian, K. Morokuma and K. Morokuma, *"Early Stages in the Nucleation Process of Carbon Nantoubes: Density-Functional Tight-Binding Molecular Dynamics Simulations of Acetylene Polymerization and Cross-Linking on an Fe_{38} Particle"*
46. December 1, 2009: 23rd Annual Meeting of the Molecular Simulation Society of Japan, Nagoya Institute of Technology, Nagoya, Japan: **S. Irle**,*"Density-functional tight-binding molecular dynamics simulations of carbon nanotube formation"*
47. November 30–December 2, 2009: The Molecular simulation Society of Japan, Nagoya, Japan: **Y. Wang**, Atsushi Ito, Hiroaki Nakamura, Stephan Irle, and Keiji Morokuma, *"Chemisorption of hydrogen on graphite (0001): Spin-Polarized Density functional tight-binding molecular dynamics simulations using G2MS-Drevied C-H parameters 2"*

48. September 21–24, 2009: 3rd Annual Meeting of Japan Society for Molecular Science, Nagoya University, Nagoya, Japan: **S. Irle**, *"Density-Fuctional Tight-Binding Studies of Finite-Size Hexagonal Graphite Flakes"*
49. September 21–24, 2009: Annual Meeting of Japan Society for Molecular Science 2009, Nagoya University, Japan: **Y. Wang**, Atsushi Ito, Hiroaki Nakamura, Stephan Irle, and Keiji Morokuma, *"The chemical Interactions between graphite (0001) and hydrogen atom, deuterium atom and tritium atom: Density functional tight-binding molecular dynamics simulation of using optimized C-H parameters"*
50. September 21–24, 2009: Annual Meeting of Japan Society for Molecular Science, Nagoya University, Nagoya, Japan: **J. Wang**, S. Irle, and K. Morokuma, *"Molecular and Electronic Structures of Di-erbium and Di-erbium-carbide Metallofullerenes $Er_2(C_2)@C_{82}$: Density Functional Theory Calculations"*
51. March 27–31, 2009: The 89th Annual Spring Meeting, Chemical Society of Japan, Nihon University, Chiba, Japan: **K. Nagura**, C.-H. Zhao, A. Wakamiya, S. Irle, S. Yamaguchi, *"Fluorescence Properties of Laterally Boryl-Substituted Nonplanar Oligoarenes"*
52. January 13, 2009: 6th FIFC Seminar, Fukui Institute for Fundamental Chemistry, Kyoto University, Japan: **B. Saha**, S. Irle, and K. Morokuma, *"Fullerene self-assembly during combustion: DFTB MD simulations"*
53. November 15, 2008: Results Meeting, Kansai Seminar House, Kyoto: *"Quantum Chemical Investigation of Dispersion Interaction in Multilayer Carbon Onions and Nanotubes",* JSPS Priority Area "Molecular Theory for Real Systems"
54. November 9, 2008: 32nd Chubu CSJ Regional Meeting, Nagoya University, Nagoya, Japan: *"Continued Growth of Single-Walled Carbon Nanotubes on Iron Catalyst Particles in Density-Functional Tight-Binding Molecular Dynamics"*
55. September 24–27, 2008: Annual Meeting of the Japan Society for Molecular Science 2008, Fukuoka, Japan: **Y. Okamoto**, Y. Ohta, S. Irle, and K. Morokuma, *"Theoretical Studies of the Role of Metal Particles for Single-Walled Carbon Nanotube Formation"*
56. September 24–27, 2008: Annual Meeting of the Japan Society for Molecular Science 2008, Fukuoka, Japan: **Y. Ohta**, Y. Okamoto, S. Irle, and K. Morokuma, *"Continued Growth of Single-Walled Carbon Nanotube by Density-Functional Tight-Binding Molecular Dynamics"*
57. March 26–30, 2008: The 88th Annual Spring Meeting, Chemical Society of Japan, Rikkyo University, Tokyo, Japan: **S. Irle,** *"DFTB/MD simulations of graphite layer healing using erosion mitigating agents"*
58. March 15–16, 2008: JSPS Priority Area "Molecular Theory for Real Systems", Results Meeting, Okayama University, Okayama, Japan: **S. Irle,** *"Performance and Application of the* A Posteriori *London-Approach for the Description of Dispersion Interaction in Carbon Nanotubes"*
59. September 16–20, 2007: Annual Meeting of the Japan Society for Molecular Science 2007, Sendai, Japan: **B. Saha**, S. Irle, and K. Morokuma, "*Quantum Chemical Molecular Dynamics Simulations of Fullerene Self-Assembly from Benzene"*
60. September 16–20, 2007: Annual Meeting of the Japan Society for Molecular Science 2007: **S. Irle,** *"Rapid Heating Transformation of Nanodiamonds to Carbon Spiroids and Onions in Quantum Chemical Molecular Dynamics Simulations"*
61. May 14–16, 2007: 10th Theoretical Chemistry Symposium, Nagoya University, Japan: **S. Irle,** *"DFTB-D Modeling of Metalized DNA: An Introduction"*
62. March 25–28, 2007: The 87th Annual Spring Meeting, Chemical Society of Japan, Kansai University, Osaka, Japan: **S. Irle,** *"Quantum Chemical Study of Oxidative High-Temperature Graphite Erosion: Dynamics, Transition Path Sampling, and ONIOM Calculations"*
63. November 2003: SERMACS 55th Regional ACS Meeting, University of Georgia, Atlanta, U.S.A.: **S. Irle,** *"From C_2 Molecules to Self-Assembled Fullerenes in High-Temperature Quantum Chemical Molecular Dynamics Simulations"*
64. September 1994: Austrian Chemistry Symposium, Graz, Austria: **S. Irle,** H. Lischka, "*Model calculations on polaronic and bipolaronic defects of Li doped oligothiophenes and -phenyls"*

Invited Department Lectures, Workshops, Seminar Talks, etc.

- February 7, 2018: Seminar Talk, Institute of Energy Studies, Western Washington University, Bellingham, WA, U.S.A.: **S. Irle**, *"Ultrafast electronic structure methods and applications to problems in materials sciences"*

- January 24, 2018: Seminar Talk, Department of Chemical Engineering, Tennessee Tech University, Cookville, TN, U.S.A.: **S. Irle**, *"Ultrafast electronic structure methods and applications to problems in materials and biosciences"*
- October 26, 2017: Seminar Talk, Department of Chemistry, Georgetown University, Washington, DC, U.S.A.: **S. Irle**, *"Quantum chemical studies of nanoscale materials self-assembly and physicochemical properties"*
- October 10, 2017: Seminar Talk, Multiscale Modeling and Simulations (MUMS) Center, Vanderbilt University, TN, U.S.A.: **S. Irle**, *"Approximate DFT methods for molecular and electronic structure and dynamics simulations"*
- September 20, 2017: Seminar Talk, Institute for Advanced Computational Sciences (IACS), Stony Brook University, Stony Brook, NY, U.S.A.: **S. Irle,** *"Some Problems of the Density-Functional Tight-Binding Method for Chemical Applications and Possible Solutions"*
- February 15, 2017: Department of Chemistry, Costa Rica University, San Jose, Costa Rica: **S. Irle,** *"Quantum Chemical Method for the Study of Complex Systems"*
- August 18, 2016: Bremen Center for Computational Material Sciences (BMCS), University of Bremen, Germany: **S. Irle,** *"Towards quantum chemical molecular dynamics simulations of soft materials"*
- July 7, 2016: Seminar at the Department of Chemistry, Siberian Federal University, Krasnoyarsk, Russia: **S. Irle,** *"The Power of Molecules – The Power of Computation"*
- June 20-21, 2016: *"FMO-DFTB Mini-Workshop",* Nagoya University, Japan: **S. Irle,** *"Approximate DFT Methods for Extended Systems"*
- April 18, 2016: Center for Nanophase Materials, Oak Ridge National Lab (ORNL), Oak Ridge, TN, U.S.A.: **S. Irle,** *"Recent Developments for Hierarchical Soft Materials Simulations"*
- April 12, 2016: Plasma Science & Technology Seminar, Princeton Plasma Physics Laboratory (PPPL), Princeton, NJ, U.S.A.: **S. Irle,** *"Quantum chemical molecular dynamics simulations of nanostructure self-assembly in plasma and CVD syntheses"*
- April 8 & 11, 2016: Workshop, Institute for Advanced Computational Sciences (IACS), Stony Brook University, Stony Brook, NY, U.S.A.: **S. Irle,** *"Formalism and Hands-on Application of Ultrafast Linear-scaling, Massively Parallel Quantum Chemical Methods Based on Density-functional Tight-binding (DFTB) for Computational Materials Sciences"*
- April 7, 2016: Seminar Talk, Institute for Advanced Computational Sciences (IACS), Stony Brook University, Stony Brook, NY, U.S.A.: **S. Irle,** *"Ultrafast Linear Scaling Quantum Chemical Methods: Methodology and Applications to Problems in Materials Sciences"*
- May 21, 2015: Seminar at the Department of Chemistry, Siberian Federal University, Krasnoyarsk, Russia: **S. Irle,** *"Quantum Chemistry for the Discovery of Transformative Bio-Molecules"*
- December 15–16, 2014: 4th Winter School in Quantum Chemistry, Institute of Molecular Science, Okazaki Conference Center, Okazaki, Japan: **S. Irle,** *"Density-Functional Tight-Binding Method for Complex Systems in Ground and Excited States"*
- November 17–20, 2014: AGS Intensive Course "Modern Trends in Chemical Sciences and Engineering II (Special Lecture 2014), Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan: **S. Irle,** Physical Chemistry (4 Lectures of 90 Minutes each).
- November 19, 2014: Department Seminar, Department of Chemistry, Hokkaido University, Sapporo, Japan: **S. Irle,** *"Recent methodological developments for the quantum chemical study of complex systems"*
- September 15, 2014: Seminar Talk, Technological Institute for Superhard and Novel Carbon Nanomaterials, Troitsk, Russia: **S. Irle,** *"Quantum chemical investigations of carbon nanostructures and their formation mechanisms"*
- June 26, 2014: Workshop on Metallofullerenes, Department of Physical and Inorganic Chemistry, Rovira i Virgili University, Tarragona, Spain: **S. Irle,** *"Insights from Density-Functional Tight-Binding Molecular Dynamics Simulations for the Formation Mechanism of Metallofullerenes"*
- June 16–27, 2014: Heraeus Summer School on "Computer Simulations of Thermally Exited Materials by First Principles", Jacobs University, Bremen, Germany: **S. Irle,** *"On fractional orbital occupation numbers in DFT and DFTB methods"*

- April 15, 2014: Seminar at DENSO Company, Nisshin City, Japan: **S. Irle,** *"How quantum chemistry can help industry R&D"*
- February 7, 2014: Department Seminar at the Department of Applied Chemistry, Osaka Prefecture University: **S. Irle,** *"Toward and Understanding of the Dynamics of Complex Chemical Systems"*
- September 27, 2013: Department Seminar at the School of Engineering and Science, Jacobs University, Bremen, Germany: **S. Irle,** *"Excited States of Large Molecules"*
- April 26, 2013: Department Seminar at the Department of Chemistry, College of Science, Ibaraki University, Mito, Japan: **S. Irle,** *"Theoretical studies of complex chemical reactions and nanostructure formation mechanisms"*
- December 24–28, 2012: Lecture Series of four lectures, Institute of Theoretical and Simulational Chemistry, Academy of Fundamental and Interdisciplinary Sciences, Harbin Institute of Technology, Harbin, China: 1. Introduction to Density Functional Theory; 2. Introduction to the Density-Functional Tight-Binding (DFTB) Method; 3. Carbon Nanostructure Formation: What Can We Learn from DFTB/MD Simulations?; 4. Excited States and Photodynamics of Large Organic Molecules
- December 4, 2012: ITC Research Seminar, Institute of Textiles and Clothing, The Hong Kong Polytechnic University, Hong Kong: **S. Irle,** *"What can we learn from molecular dynamics simulations of carbon nanotube and graphene growth?"*
- November 19, 2012: GCOE for Mechanical Systems Innovation (GMSI) Seminar, The University of Tokyo, Tokyo, Japan: **S. Irle,** *"What Can We Learn from Current Molecular Dynamics Simulations of Nanotube Growth?"*
- October 24, 2012: Japan Fine Ceramics Center, Nagoya, Japan: **S. Irle,** *"Mechanism of carbon nanotube and graphene formation during high-temperature vacuum decomposition of SiC"*
- October 5, 2012: Department of Applied Chemistry, National Chiao Tung University, Hsinchu, Taiwan: **S. Irle**, *"Density-Functional Tight-Binding For the Study of Complex Chemical Reactions"*
- September 17, 2012: Center Seminar, Bremen Center for Computational Material Science (BCCMS), Bremen University, Germany: **S. Irle,** *"Quantum Chemistry of Complex Systems in Nagoya and Japan"*
- April 20, 2012: TR24 Seminar, Institute of Physics, Ernst Moritz Arndt University Greifswald, Germany: **S. Irle,** *"On the prediction of chemical reaction pathways and reaction rates in complex systems using quantum chemical MD simulations"*
- March 6, 2012: "GCOE Delegates Meeting for Participants from Malaysia and Indonesia", Nagoya University, Japan: **S. Irle**, *"Quantum Chemistry of Complex Systems"*
- February 20, 2012: "Joint Seminar on Science and Technology", NanoCarbon Research Institute, Ueda, Japan: **S. Irle**, "A priori *prediction of chemical reaction pathways in complex systems: Metallofullerene formation and related systems"*
- February 20, 2012: "Joint Seminar on Science and Technology", NanoCarbon Research Institute, Ueda, Japan: **Y. Nishimoto**, S. Irle, *"Molecular and electronic structures of transition metal clusters: Endohedral metallofullerenes and polyoxometalate clusters"*
- February 13, 2012: Department of Chemistry Seminar, Yokohama City University, Yokohama, Japan: **S. Irle,** *"Quantum chemical molecular dynamics simulations of graphene hydrogenation"*
- December 29, 2011: Department of Applied Chemistry, National Chiao Tung University, Hsinchu, Taiwan: **S. Irle**, *"Fun with graphenes: quantum chemical simulations of formation and hydrogenation dynamics"*
- October 18, 2011: Department Seminar, Computational Chemistry Unit Cell, Department of Chemistry, Chulalongkorn University, Thailand, **S. Irle,** Y. Wang, Y. Nishimoto, H.-J. Qian, A. J. Page, K. Morokuma, *"Fun with graphenes: quantum chemical simulations of formation and hydrogenation dynamics"*
- October 17, 2011: Special Department Seminar, Department of Chemistry, Kasetsart University, Bangkok, Thailand, **S. Irle**, Y. Nishimoto, Benjamin Finck, Z. Wang, Keiji Morokuma, *"New Insights from Quantum Chemical Molecular Dynamics Simulations on the Formation Mechanism of Metallofullerenes"; "Computational chemistry with the role of a dice: stochastic structure generation from metal clusters to ionic liquids"*
- October 10–12, 2011: Second Annual EPSCoR Workshop: Modeling Advanced Materials, Systems Biology, and Alternative Energy Sources, University of Tennessee, Knoxville, TN, U.S.A.: **S. Irle,**

"Haeckelite and Graphene Formation on a Metal Surface: Evidence for a Phase Transformation at the Edge of Criticality"

- July 3–15, 2011: Heraeus Summer School on "Nanotechnology for the environment: New nanomaterials, their applications and new simulation methods", Jacobs University, Bremen, Germany, *"DFT in the heat: DFT-based molecular dynamics for thermally and optically excited systems"* (2 lectures)
- March 15, 2011: Seminar at the Department of Chemistry, Siberian Federal University, Krasnoyarsk, Russia: invited: *"DFT-based simulations of thermally and optically excited nanomaterials"*
- March 7, 2011: One Day Workshop on Physical Chemistry of Nano-Structured Materials, RCMS, Nagoya University, Nagoya, Japan: *"Graphene hydrogenation: Band gap tuning and the discovery of C_4H, a new polymer"*
- January 27, 2011: Nanosystem Research Institute, AIST, Tsukuba, Japan, *"Density-Functional Tight-Binding: Theory and Recent Developments"*
- January 26, 2011: Nanotube Research Center, AIST, Tsukuba, Japan, *"New quantum chemical MD simulations of nanocarbon structure formation"*
- December 2, 2010: Department of Physics, Göteborg University, Sweden, **S. Irle,** *"Fullerenes, nanotubes, graphenes: insights for synthesis from theory"*
- June 14, 2010: Department of Chemistry, Tohoku University, Sendai, Japan, **S. Irle**, *"Laser heating, collisions, and coalescence of functionalized fullerenes"*
- June 8, 2010: L. Kirensky Institute of Physics, Russian Academy of Sciences, Krasnoyarsk, **KRS Chandrakumar,** S. Irle, and K. Morokuma, *"Growth of Nanotubes/Nanocapsules from Metal Decorated Carbon Nanocone Aggregates: Insights from DFTB/MD Simulations"*
- June 7, 2010: L. Kirensky Institute of Physics, Russian Academy of Sciences, Krasnoyarsk, **S. Irle,** *"Graphene: molecular structure, vibrational spectroscopy, and hydrogen adsorption"*
- April 16, 2010: Seminar Talk, Department of Chemistry, Florida International University, Miami, FL, U.S.A., B. Saha, S. Shindo, **S. Irle**, K. Morokuma*"Quantum chemical MD simulations of combustion fullerene synthesis"*
- April 14, 2010: Seminar Talk, CMSD, Oak Ridge National Labs, Oak Ridge, TN, U.S.A., *"Electronic structure theory and the simulation of emergent phenomena on the nanoscale"*
- April 13, 2010: Seminar Talk, Center for Nanophase Materials Sciences, Oak Ridge National Labs, Oak Ridge, TN, U.S.A. *"Quantum chemical MD simulations of metal-catalyzed SWNT growth and SWNH transformations"*
- April 12, 2010: Seminar Talk, Department of Chemistry, Middle Tennessee State University, Murfreesboro, TN, U.S.A.: *"Quantum chemical studies of carbon nanotube formation and IR stealth effect in nanotube sensors"*
- March 11, 2010: Institute for Molecular Science (IMS), Okazaki, Japan: **L. Liu**, S. Irle, *"DFTB investigations of finite-size graphene flakes and their vacancy defects: structures and dynamics"*
- March 8, 2010: International Workshop on Organic Electronics and Spintronics, Meitetsu Hotel, Nagoya, Japan: *"Quantum chemical molecular dynamics simulations of SWNT nucleation and growth on iron and nickel"*
- December 17, 2009: Department of Simulation Science, NIFS, Toki, Gifu, Y. Wang, A. Ito, H. Nakamura, K. Morokuma, and **S. Irle** *"Comparison of classical and quantum chemical molecular dynamics simulations of hydrogen chemical sputtering on graphite"*
- December 2, 2009: GCOE for Mechanical Systems Innovation (GMSI) Seminar, The University of Tokyo, Tokyo, Japan: invited: *"Quantum Chemical Molecular Dynamics Simulations of SWNT Nucleation and Growth on Iron and Nickel"*
- November 26, 2009: Seminar at the Computational/Theory Group at National Chiao Tung University, Hsinchu, Taiwan: invited: *"Quantum chemical molecular dynamics simulations of fullerene and carbon nanotube formation"*
- November 24, 2009: Global MBA Program, National Chiao Tung University, Hsinchu, Taiwan: invited: *"Globalization from a Science and Technology Perspective"*
- November 16, 2009: Global COE Seminar at the Department of Physics, Tokyo Institute of Technology, Tokyo, Japan: invited: *"Quantum chemical molecular dynamics simulations of fullerene and carbon nanotube formation"*

- September 14, 2009: Seminar at the Nanotube Research Center, National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan: invited: *"Quantum chemical investigations of pristine and defective graphene flakes"*
- September 8, 2009: Seminar at the Department of Chemistry, Siberian Federal University, Krasnoyarsk, Russia: invited: *"Quantum chemical molecular dynamics study of structure, electronic properties, and growth mechanisms of carbon-based nanoclusters"*
- July 31, 2009: Department of Scientific and Engineering Simulation, Nagoya Institute of Technology, Nagoya, Japan: invited: *"Quantum Chemical Molecular Dynamics Simulations of Fullerene Formation during Benzene Combustion"*
- June 23, 2009: State Key Laboratory of Theoretical and Computational Chemistry, Jilin University, Changchun, China: invited: *"Density-Functional Tight-Binding Studies of Hexagonal Graphite Flakes, Defect Formation, and Hole Healing"*
- June 22, 2009: State Key Laboratory of Theoretical and Computational Chemistry, Jilin University, Changchun, China: invited: *"C_{60} & Company "made" by quantum chemical molecular dynamics"*
- May 21, 2009: Emerson Center Special Seminar, Emory University, Atlanta, GA, U.S.A.: invited: *"Density-Functional Tight-Binding Studies of Hexagonal Graphite Flakes, Defect Formation, and Hole Healing"*
- April 16, 2009: NanoCenter at the University of South Carolina, Columbia, SC, U.S.A.: invited: *"C_{60} & Company "made" by quantum chemical molecular dynamics",* Seminar on Nanoscale Theory, Modeling and Simulation,
- February 3–8, 2009: the Sokdendai Asian Winter School "Science of Fluctuations and Structure Formation – Life, Material, and Space", http://www.dss.nifs.ac.jp/aws/ National Institute for Fusion Science (NIFS), Toki, Japan: invited: *"Theory and Applications of Quantum Chemical Molecular Dynamics Simulations of Plasma Processes"*
- January 27, 2009: invitation by the International Research Training Group (IRTG) Leader Prof. Gerhard Erker, Munster, Germany: invited seminar: *"Continued Growth of Single-Walled Carbon Nanotubes on Iron Catalyst Particles in Density-Functional Tight-Binding Molecular Dynamics"*
- January 26, 2009: invitation by the International Research Training Group (IRTG), University of Munster, Germany, Leader: Prof. Gerhard Erker: invited workshop: *"Theory and Applications of Quantum Chemical Molecular Dynamics Simulations of High-Temperature Reaction Environments"*
- January 23, 2009: Department of Chemistry, University of Siegen, Germany, invitation by Prof. W. H. Eugen Schwarz: invited seminar: *"Continued Growth of Single-Walled Carbon Nanotubes on Iron Catalyst Particles in Density-Functional Tight-Binding Molecular Dynamics"*
- November 28, 2008: Department of Chemistry, Okayama University, invitation by Prof. Kubosono: invited: *"Continued Growth of Single-Walled Carbon Nanotubes on Iron Catalyst Particles in Density-Functional Tight-Binding Molecular Dynamics"*
- November 14, 2008: Friday Workshop on Organic Electronics, Presidential Discretionary Funding Research Meeting, Department of Chemistry, Nagoya University, invitation by Prof. Awaga: invited: *"DFTB Parameter Development: Towards Ab Initio Quality Hydrogen-Graphite MD Simulations"*
- July 3, 2008: Department of Chemistry, University of Hawaii at Manoa, Honolulu, HI, U.S.A.*: "Performance and Application of the* A Posteriori *London-Approach for the Description of Dispersion Interaction in Carbon Nanotubes"*
- June 11, 2008: Global-COE workshop on "Elucidation and Design of Materials and Molecular Functions", Nagoya, Japan: *"Quantum Chemical Modeling of Carbon Nanotubes: From Formation Mechanisms to Applications"*
- May 30, 2008: invitation by Prof. Henryk Witek for the Department of Chemistry, National Chiao Tung University, Hsinchu, Taiwan: *"C_{60} & Company made by quantum chemical molecular dynamics"*
- March 18, 2008: Workshop organized by Kochi Sasaki, Plasma Nanotechnology Research Center, Nagoya University, Nagoya, Japan: **Y. Wang**, S. Irle, and K. Morokuma, "Ab Initio *and Density Functional Theory Potential Energy Curves for the Reaction of Atomic Hydrogen With Coronene and Pyrene"*
- March 18, 2008: invitation by Prof. Koichi Sasaki, Plasma Nanotechnology Research Center, Nagoya University, Nagoya, Japan: *"Quantum Chemical Molecular Dynamics Studies of Emergent Structure Formation in Nanocarbon Systems under Extreme Conditions"*

- March 17, 2008: Global-COE workshop on "New Concepts and Materials for Molecular Electronics and Magnetism", Nagoya, Japan: Invited Talk: *"Quantum Chemical Molecular Dynamics Studies of Emergent Structure Formation in Nanocarbon Systems under Extreme Conditions"*
- February 7, 2008: invitation by Dr. Gyula Eres, Center for Nanophase Materials, Oak Ridge National Lab (ORNL), Oak Ridge, TN, U.S.A.: *"Dynamics of Carbon Nanotube Self-Assembly Using Quantum Chemical Potential"*
- October 30, 2007: invitation by Prof. Masataka Nagaoka, Graduate School of Information Science, Nagoya University, Nagoya, Japan: *"Quantum Chemical Molecular Dynamics Simulations of Dynamic Self-Assembly and Erosion Processes under Extreme Conditions"*
- August 25, 2007: invitation by Prof. Jack Howard (MIT) to Nano-C, Inc., Boston, MA, U.S.A.: *"Quantum Chemical Molecular Dynamics Simulations of Fullerene During Benzene Combustion"*
- April 25, 2007: Invitation to Physical Chemistry Seminar "Dynamical Aspects of Carbon sp/sp^2 Hybrid Systems", Department of Chemistry, Kinki University, Osaka, Japan: *"Quantum Chemical Molecular Dynamics Simulations of Fullerene and Carbon Nanotube Formation"* and *"Prediction of Isomer Geometries of Polyyne@SWNT Peapods Using Dispersion-Augmented Density-Functional Tight-Binding"*
- April 13, 2007: invitation for a Cherry L. Emerson Center for Scientific Computation Special Seminar at Emory University, Atlanta, GA, U.S.A.: *"Quantum Chemical Molecular Dynamics Simulations of Fullerene and Carbon Nanotube Formation and Graphite Erosion Processes"*
- January 2007: invitation to JST/CREST meeting organized by Prof. Takeo Fujiwara, Department of Applied Physics, Tokyo University, Tokyo, Japan*:"Recent progress in quantum chemical simulations of nanomaterials"*
- January 2007: Department of Physics, Kyoto University, Kyoto, Japan: *"Quantum Chemical Molecular Dynamics Simulations of Fullerene and Carbon Nanotube Self-Assembly"*
- August 2006: Nagoya University and Japan Fine Ceramics Center, Nagoya, Japan: *"Quantum Chemical Molecular Dynamics Simulations of Metallofullerene Formation and Carbon Nanotube Nucleation Processes"*
- August 2006: Computational Chemistry Unit Cell, Chulalongkorn University, Bangkok, Thailand: *"The Nucleation Process of Carbon Nanotubes Studied by QM/MD Simulations"*
- May 2005: 3rd Fukui Center Seminar, Fukui Institute for Fundamental Chemistry, Kyoto, Japan*: "QM/MD simulations of high-temperature CNT growth on SiC surfaces"*
- April 2006: Oak Ridge National Laboratory, Center for Computational Sciences (CCS) and Center for Nanophase Materials Sciences (CNMS), Oak Ridge, Tennessee, U.S.A.: *"DFTB-based QM/MD simulations of nanostructure formation processes far from thermodynamic equilibrium"*
- October 2005: Japan Fine Ceramics Center, Nagoya: *"Theory and Experiment Agree: SWNT Caps Grow Catalyst Free with Chirality Preference on SiC Surfaces"*
- October & November 2005: Nagoya University; Ochanomizu University, Tokyo; Research Institute for Computational Sciences and Research Center for Advanced Carbon Materials, AIST, Tsukuba; Fundamental and Environmental Research Laboratories, NEC Corporation, Tsukuba; Center for Nanotubes and Nanostructured Composites (CNNC), Sungkyunkwan University, Seoul; University of Tokyo; Mitsubishi Frontier Carbon Corporation, Yokohama; Yokohama City University; Institute for Molecular Science (IMS), Okazaki; Tohoku University, Sendai: Series of 3 Lectures at various locations in Japan and Korea: *"Achieving Control over SWNT Functionalization and Adsorptivity"*, *"QM/MD Simulations and PES Landscapes of Fullerene Formation"*, *"Nucleation and Growth of SWNTs Studied by QM/MD Simulations"*
- September 2005: Oak Ridge National Laboratory, Center for Computational Sciences (CCS) and Center for Nanophase Materials Sciences (CNMS), Oak Ridge, Tennessee, U.S.A.: *"Fe/C Interactions During SWNT Growth with C_2 Feedstock Molecules: A Quantum Chemical Molecular Dynamics Study"*
- August 2004: Nagoya University, Nagoya, Japan: *"Order Out of Chaos: Computer Simulations of High-T Carbon"*
- July 2004: University of Paderborn, Germany: *"Applications of ONIOM in nanotechnology with emphasis on the DFTB method"*

- June 2003: University of Tokyo, NanoCarbon Research Institute Limited, Chiba, and Mitsubishi Chemical Corporation, Yokohama, Japan: *"Order out of chaos: The role of quantum mechanics in carbon nanochemistry"*
- April 2002: University of Puerto Rico, San Juan, U.S.A.: "*New technical evolution of the ONIOM method and applications to problems in nanotechnology*"
- September 2001: Universities of Tokyo and Kyoto, Mitsubishi Chemical Corporation, Yokohama, and RIKEN, Saitama, Japan: *"Applications of ONIOM in nanotechnology: Prediction of structures and spectra of nanotubes and nanoclusters"*
- April 1998: School for Biochemistry and Chemistry, Georgia Institute of Technology, Atlanta, Georgia, U.S.A.: *"Quantum Chemical Model Calculations on Ion Molecule Reactions and Conducting Polymers"*
- October 1996: Austrian Thai Center for Computer Chemistry, Chulalongkorn University, Bangkok, Thailand: *"Density Functional Theory in comparison with conventional* ab initio *methods and recent results on conducting polymers"*

TEACHING EXPERIENCE

- Spring semester, 2014 and 2015: Undergraduate Course "Quantum Chemistry III" for junior level students in English, Nagoya University, Japan. Part of the Nagoya University G30 program.
- Fall semester, from 2011 – 2017: Undergraduate Course "Computational Chemistry" for junior level students in Japanese and English, Nagoya University, Japan. Part of the Nagoya University G30 program.
- Fall semester, from 2007 – 2014: Graduate Course "Advanced Quantum Chemistry: Molecular Dynamics Simulations in Highly Reactive Environments", Department of Chemistry, University of Nagoya, Japan
- Summer semester, from 2007 – 2014: Special Undergraduate Course "Self-Assembly Mechanisms in Nature", 6 lectures for 2nd year undergraduate students in English, Department of Chemistry, University of Nagoya, Japan
- Fall semester, from 2005 – 2017: Special Graduate Course "Introduction to Computational Chemistry", Department of Chemistry, University of Nagoya, Japan.
- Fall 2003, Spring 2004, Fall 2005: Substitute Lecturer for several hours of CHEM533, CHEM532, and CHEM531, Department of Chemistry, Emory University, Atlanta, Georgia, U.S.A.
- Spring 1999, 2001, and 2003: Special Short Course on Practical Computational Chemistry, Cherry L. Emerson Center for Scientific Computation, Emory University, Atlanta, Georgia, U.S.A.

POSTDOCS SUPERVISED (18 as independent PI)

1. Winter 2016 – Winter 2017: Dr. Christin Rakers, PhD: Humboldt University, Germany. Research topic: "Studies of Striga suicide germination mechanisms".
2. Spring 2016 – Summer 2017: Dr. Shingo Ito, PhD: Nagoya University. Research topic: "Replica exchange MD simulations with DFTB".
3. Fall 2016 – Spring 2017: Dr. Supriya Saha, PhD: Visva-Bharati University, India. Research topic: "DFTB parameterization of metal alloys in combination with CHON elements".
4. Spring 2016 – Spring 2017: Dr. Li-Xia Zhao, PhD: East China University of Science and Technology, Shanghai, China. Supported by the Shanghai Education Committee. Research topic: "Unraveling Special Effects of Transition Metal Atoms in the Core of Gold Nanoparticles".
5. Spring 2014 – Fall 2017: Dr. Kai Welke, PhD: Karlsruhe Institute of Technology, Germany. From Fall 2015: JSPS-AvH Fellowship. 2 papers published. Research topics: FMO-DFTB, biosimulations, XL-BOMD.
6. Summer 2013 – Spring 2016: Dr. Anupriya Kumar, PhD: Pohang University of Science and Technology, Pohang, South Korea. 2 papers published, 1 corresponding author paper. Research topics: Binding free energy calculations of molecules with proteins; docking simulations, QSAR. Present position: Designated Assistant Professor, Graduate School of Medicine, Nagoya University.
7. Spring 2013 – Spring 2016: Dr. Hirotaka Kitoh-Nishioka, PhD: Nagoya University. Research topics: Calculations of fluorescence resonance energy transfer; fragment molecular orbital method development. 1 paper published. Research topics: Method development for excitation energy and electron transfer, QM/MM simulations. Present position: Postdoc, Tsukuba University.

8. Spring – Fall 2015: Dr. Arthithaya Meeprasert, PhD: Chulalongkorn University. Visiting from Chulalongkorn University. Research topics: Classical biosimulations, QM/MM simulations.
9. Fall 2012 – Spring 2015: Dr. Vennapusa Sivaranjana Reddy, PhD: University of Hyderabad, India. 1 first-author paper published. Research topics: Quantum nuclear dynamics of large molecules in excited states. Present position: Assistant Professor, Indian Institute of Science Education and Research Thiruvananthapuram.
10. Fall 2013 – Spring 2014: Wichien Sang-aroon, PhD: Chulalongkorn University, Thailand. Visiting from Rajamangala University of Technology Isan, Khonkaen, Thailand. Research interests: Simulations of molecules in excited states.
11. Spring 2014: Dr. Auradee Punkvang, PhD: Ubon Ratchathani University, Thailand. Visiting from Nakhon Phanom University, Thailand. 2 papers published, 1 first-author paper. Research topics: QSAR, classical biosimulations, QM/MM simulations.
12. Fall 2012 – Spring 2014: Dr. Tim Kowalzcyk, PhD: Massachusetts Institute of Technology (MIT), Boston, MA, U.S.A. JSPS postdoctoral fellow. 4 papers published, 1 first-author paper. Research topics: Method development for excited states of large molecules. Present position: Assistant Professor, Western Washington University.
13. Spring 2011 – Spring 2013: Dr. Cristopher Camacho Leandro, PhD: National Chiao Tung University, Taiwan. 7 papers published, 1 first-author paper. Research topic: Dynamics and properties of large molecules in excited states. Present position: Associate Professor, Costa Rica University.
14. Winter 2010 – Fall 2012: Dr. Matthew Addicoat, PhD: University of Adelaide, Australia. JSPS-AAS postdoctoral fellow. 14 papers published, 3 first-author papers. Research topics: Simulation of ionic liquids on polarizable surfaces; covalent organic frameworks. Present position: Research of the Volkswagen Foundation, University of Leipzig.
15. Spring – Fall 2012: Dr. Gabriele Manca, PhD: University of Pisa, Italy. Visiting from Instituto di Chimica dei Composti Organometallici (ICCOM), Florence, Italy. Research topics metal clusters, DFT.
16. Fall 2007 – Spring 2011: Dr. Ying Wang, PhD: Jilin University, China. 21 papers published, 4 first-author papers. Research topic: Molecular dynamics simulations of nanoscale materials. Present position: Associate Professor, Chinese Academy of Science, Changchun.
17. Summer 2011: Dr. Oraphan Saengsawang. PhD: Chulalongkorn University, Bangkok, Thailand. Visiting for 1 month. 1 paper published. Research topic: Molecular and electronic structure of Covalent Organic Frameworks (COFs). Present position: Researcher, IRPC Public Company Limited, Bangkok, Thailand.
18. Spring 2008 – Spring 2011: Dr. Hu-Jun Qian, PhD: Jilin University, China. 9 papers published, 1 first-author paper. Research topic: Molecular dynamics simulations of nanoscale materials. Present position: Associate Professor, Jilin University.
19. Spring 2009 – March 2011: Dr. Jian Wang, PhD: Jilin University, China. 4 papers published, 1 first-author paper. Research topic: Excited states of large molecules & DFT calculations of metallofullerenes. Present position: Postdoc, Hong Kong Polytechnic University.

Co-supervised with Prof. Keiji Morokuma on a JST/CREST grant or Fukui fellow, Kyoto University:

20. Fall 2010 – Summer 2012: Dr. Joonhan Kim (Fukui Fellow) (present position: postdoc, Catholic University in Seoul)
21. Summer 2010 – Fall 2013: Dr. Hai-Bei Li (JST/CREST) (present position: Assistant Professor, Shandong University, China)
22. Winter 2008/2009 – Fall 2013: Dr. Alister Page (JST/CREST, later Fukui Fellow) (present position: Permanent Lecturer, The University of Newcastle, Australia)
23. Spring 2009 – Spring 2011: Dr. KRS Chandrakumar (JST/CREST) (present position: lecturer, IIT Bombay, India)
24. Fall 2009 – Spring 2010: Dr. Pattiyil Parameswaran (JST/CREST) (present position: lecturer, India)
25. Spring 2008 – Spring 2009: Dr. Tom Grimes (JST/CREST)
26. Fall 2006 – Spring 2010: Dr. Biswajit Saha (Fukui Fellow) (present position: Assistant Professor, Amity University, India)
27. Fall 2006 – Spring 2009: Dr. Yasuhito Ohta (JST/CREST) (present position: Associate Professor, Nara Women's University)
28. Fall 2006 – Fall 2009: Dr. Yoshiko Okamoto (JST/CREST)

Co-supervised with Prof. Keiji Morokuma, Emory University:

29. Before 2006: Dr. Antara Dutta
30. Before 2006: Dr. Vencislav Parvanov
31. Before 2006: Dr. Henryk Witek (present position: Professor, National Chiao Tung University, Hsinchu, Taiwan)

GRADUATE STUDENTS SUPERVISED (10 members of my group, 30 visiting or co-supervised)

1. Fall 2016 – present: Ka Hung Lee, Department of Chemistry, Nagoya University, since 2017: Bredesen Center, University of Tennessee Knoxville, U.S.A.
2. Fall 2016 – present: Quan V. Vuong, Department of Chemistry, Nagoya University, since 2017: Bredesen Center, University of Tennessee Knoxville, U.S.A.
3. Fall 2015 – Spring 2018: Longtao Han, Institute of Advanced Computational Sciences, Stony Brook University, U.S.A.
4. Spring 2014 – present: Mr. Taku Hayashi, Department of Chemistry, Nagoya University, Japan.
5. Fall 2013 – Fall 2017: Mr. Aulia Sukma Hutama, Institute of Technology, Bandung, Indonesia (G30 fellow)
6. Fall 2012 – Fall 2016: Mr. Arifin, Institute of Technology, Bandung, Indonesia (G30 fellow)
7. Spring 2012 – Spring 2016: Dr. Kosuke Usui, Department of Chemistry, Nagoya University (present position: Kobayashi Pharmaceutical Co., Ltd., Osaka, Japan).
8. Fall 2015: Mr. Junda Li, visiting from Department of Chemistry, University of Adelaide, Australia.
9. Spring – Fall 2015: Mr. Chanchai Sattayanon, visiting from Chiang Mai University, Thailand.
10. Spring – Summer 2015: Mr. Mathias Piescheck, visiting from the Braunschweig University of Technology, Germany.
11. Spring – Summer 2015: Mr. Izaac Mitchel, visiting from The University of Newcastle, Australia.
12. Spring – Winter 2015: Ms. Jenny Pirello, visiting from the University of Calabria, Italy
13. Fall 2014 – Fall 2015: Mr. Rathawat Daengngern, visiting from Chiang Mai University, Thailand.
14. Spring 2013 – Spring 2015: Mr. Naoto Baba, Department of Chemistry, Nagoya University
15. Fall 2014 – Spring 2015: Mr. Ruangchai Tarsang, visiting from Ubon Ratchathani University, Thailand.
16. Fall 2014 – Spring 2015: Ms. Evgeniia Kovaleva, visiting from Siberian Federal University, Krasnoyarsk, Russia.
17. Summer 2014 – Spring 2016: Dr. Shingo Ito (co-supervision with Prof. Yuko Okamoto), visiting from Department of Physics, Graduate School of Science, Nagoya University (present position: postdoctoral fellow, Nagoya University)
18. Spring – Fall 2014: Mr. Pharit Kamsri, visiting from Ubon Ratchathani University, Thailand.
19. Fall 2013 – Spring 2014: Mr. Qingming Deng, visiting from Leibniz Institute for Solid State and Materials Research (IFW), Germany.
20. Spring – Summer 2013: Ms. Yaowarat Surakhot, visiting from Ubon Ratchathani University, Thailand.
21. Spring – Summer 2013: Mr. Rathawat Daengngern, visiting from Chiang Mai University, Thailand.
22. Spring – Fall 2012: Ms. Chonpoonut Rungnim, visiting from Department of Chemistry Chulalongkorn University, Bangkok, Thailand.
23. Spring 2010 – Spring 2013: Mr. Noriyuki Ogasawara (co-supervision with Prof. Michiko Kusunoki), Ecotopia, Nagoya University
24. Spring 2010 – Spring 2015: Dr. Yoshio Nishimoto, Department of Chemistry, Nagoya University (present position: Fukui Fellow at the Fukui Institute of Fundamental Chemistry, Kyoto University)
25. Spring 2009 – Spring 2012: Dr. Kazuhiko Nagura (co-supervision with Prof. Shigehiro Yamaguchi), Department of Chemistry, Nagoya University
26. Fall 2008 – Spring 2012: Dr. Lili Liu, Department of Chemistry, Nagoya University (present position: postdoctoral fellow in Beijing, China)
27. Spring 2008 – Spring 2013: Dr. Yoshifumi Nishimura, Department of Chemistry, Nagoya University (present position: postdoctoral fellow at Waseda University, Japan)
28. Spring – Summer 2011: Ms. Elena A. Vishnyakova, visiting from Siberian Federal University, Krasnoyarsk, Russia
29. Spring 2011: Mr. Danny Haberer, visiting from the University of Vienna, Austria.

30. Summer 2009: Mr. Hung Tien Nguyen, visiting from the Institute for Computational Sciences & Technology, HCM City, Vietnam (JENESYS participant) (present position: PhD program, Rutgers University)
31. Spring 2009 – Spring 2011: Mr. Masato Morita (co-supervision with Prof. Michiko Kusunoki), Ecotopia, Nagoya University (present position: Chemical Industry, Japan)
32. Spring 2009 – Spring 2011: Mr. Hironori Hara, Department of Chemistry, Nagoya University (present position: Transportation Industry, Shizuoka)
33. Summer 2010: Dr. Chatchawal Wongchoosuk, visiting from Mahidol University, Bangkok, Thailand (JENESYS participant) (present position: lecturer, Mahidol University, Bangkok, Thailand)
34. Summer 2008: Mr. Wun-Fan Li, Department of Chemistry, Nagoya University, visiting from Department of Applied Chemistry, National Chiao Tung University, Hsinchu, Taiwan (present position: postdoctoral fellow at the Free University of Amsterdam, The Netherlands)
35. Spring 2008: Dr. Genki Ichinose, Department of Complex Systems Science, Nagoya University (visiting Irle lab) (present position: Assistant Professor, Anan National College of Technology, Tokushima, Japan)
36. Spring 2007 – Fall 2007: Mr. Chun-Hao Mou (co-supervision with Prof. Keiji Morokuma), Fukui Institute for Fundamental Chemistry, Kyoto University, visiting from Department of Applied Chemistry, National Chiao Tung University, Hsinchu, Taiwan
37. Fall 2003 – 2007: Dr. Zhi Wang (co-supervision with Prof. Keiji Morokuma), Department of Chemistry, Emory University (present position: banking industry, Hong Kong)
38. Fall 2001 – Summer 2006: Dr. Guishan Zheng (co-supervision with Prof. Keiji Morokuma), Department of Chemistry, Emory University (present position: banking industry).
39. Fall 2001 – Fall 2005: Dr. Sung J. Mo (co-supervision with Prof. Keiji Morokuma), Department of Chemistry, Emory University (present positition: lecturer at Alma College, MI).

<u>UNDERGRADUATE STUDENTS SUPERVISED</u> (26 members of my group, 13 visiting or co-supervised)

1. Summer 2018: Mr. Mouhmad H. Elyyan, Department of Chemical Engineering, Tennessee Technology University
2. Fall 2016 – Spring 2017: Mr. Ryosuke Shimizu, Department of Chemistry, Nagoya University
3. Spring 2016 – Spring 2017: Mr. Ryuto Kimura, Department of Chemistry, Nagoya University
4. Spring 2016 – Spring 2017: Mr. Shouta Nakataki, Department of Chemistry, Nagoya University
5. Spring 2016 – Spring 2017: Mr. Naoto Inai, Department of Chemistry, Nagoya University
6. Spring 2015 – Spring 2016: Mr. SeokJin Moon, Department of Chemistry, Nagoya University, visiting for 12 months from Seoul National University, Korea under the Campus Asia program.
7. Fall 2014 – Fall 2015: Mr. Rafael Souza Mattos, Department of Chemistry, Nagoya University, visiting for 12 months from the Federal University of Rio de Janeiro, Brazil under a Brazilian Program "Science without borders", an undergraduate sandwich program.
8. Spring 2015 – Spring 2016: Mr. Katsuhiro Ito, Department of Chemistry, Nagoya University
9. Spring 2015 – Spring 2016: Mr. Naohiro Obata, Department of Chemistry, Nagoya University (present position: Resorttrust, Nagoya, Japan).
10. Summer 2015: Ms. Chonnikan "Kungking" Hanpaibool, Department of Chemistry, Nagoya University, visiting from Mahidol University, Bangkok, Thailand
11. Fall 2014 – Fall 2015: Ms. Raashida Tan, Department of Chemistry, Nagoya University, G30 program.
12. Spring 2014– Spring 2015: Mr. Yasumasa Namba, Department of Chemistry, Nagoya University
13. Spring 2014 – Spring 2015: Mr. Mikinori Ando, Department of Chemistry, Nagoya University
14. Spring 2014 – Spring 2015: Mr. Ryotaro Yamada, Department of Chemistry, Nagoya University
15. Spring 2013 – Spring 2014: Mr. Yuya Akao, Department of Chemistry, Nagoya University
16. Spring 2013 – Spring 2014: Mr. Masachika Kato, Department of Chemistry, Nagoya University
17. Spring 2013 – Spring 2014: Ms. Mari Shibata, Department of Chemistry, Nagoya University
18. Spring 2012 – Spring 2013: Mr. Naoto Baba, Department of Chemistry, Nagoya University
19. Spring 2012 – Spring 2013: Mr. Jun Kato, Department of Chemistry, Nagoya University
20. Spring 2011 – Spring 2012: Mr. Shinsuke Iwata, Department of Chemistry, Nagoya University
21. Spring 2011 – Spring 2012: Ms. Ayaka Ban, Department of Chemistry, Nagoya University
22. Spring 2011 – Spring 2012: Mr. Syou Fukuoka, Department of Chemistry, Nagoya University
23. Spring 2010 – Spring 2011: Mr. Ryota Umeda, Department of Chemistry, Nagoya University

24. Spring 2010 – Spring 2011: Mr. Kousuke Usui, Department of Chemistry, Nagoya University
25. Spring 2010 – Spring 2011: Mr. Yoshitaka Okita, Department of Chemistry, Nagoya University
26. Spring 2009 – Spring 2010: Mr. Yoshio Kato, Department of Chemistry, Nagoya University
27. Spring 2009 – Spring 2010: Mr. Yoshio Nishimoto, Department of Chemistry, Nagoya University
28. Spring 2009 – Spring 2010: Mr. Takahisa Fujimori, Department of Chemistry, Nagoya University
29. Spring 2008 – Spring 2009: Mr. Hironori Hara, Department of Chemistry, Nagoya University
30. Spring 2008 – Spring 2009: Mr. Kazuhiko Nagura (co-supervised with Prof. Shigehiro Yamaguchi), Department of Chemistry, Nagoya University
31. Fall 2007 – Summer 2009: Mr. Tirth Patel (co-supervised with Prof. Keiji Morokuma), Cherry L. Emerson Center for Scientific Computation and Department of Chemistry, Emory University
32. Fall 2007 – Spring 2012: Mr. Sho Shindo (co-supervised with Prof. Keiji Morokuma), Fukui Institute for Fundamental Chemistry, Kyoto University
33. Spring 2007 – Spring 2008: Mr. Yoshifumi Nishimura, Department of Chemistry, Nagoya University
34. Fall 2006 – Spring 2008: Mr. Daiki Ishida (co-supervised with Prof. Keiji Morokuma), Fukui Institute for Fundamental Chemistry, Kyoto University
35. Spring 2006 – Fall 2008: Mr. Benjamin Finck (co-supervised with Prof. Keiji Morokuma), Cherry L. Emerson Center for Scientific Computation and Department of Chemistry, Emory University
36. Fall 2003 – Summer 2005: Ms. Dovie M. Stanley (co-supervised with Prof. Keiji Morokuma), Cherry L. Emerson Center for Scientific Computation and Department of Chemistry, Emory University
37. Fall 2001 – Spring 2003: Ms. JiYeon Ku (co-supervised with Prof. Keiji Morokuma), Cherry L. Emerson Center for Scientific Computation and Department of Chemistry, Emory University
38. Spring 2001 – Summer 2001: Steven S. Shaver (co-supervised with Prof. Keiji Morokuma), Cherry L. Emerson Center for Scientific Computation and Department of Chemistry, Emory University
39. Fall 2000 – Spring 2001: Ms. Aiko Toya (co-supervised with Prof. Keiji Morokuma), Cherry L. Emerson Center for Scientific Computation and Department of Chemistry, Emory University