STEPHAN IRLE

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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, DOE, 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).
- **Fellow**, American Association for the Advancement of Science (AAAS), October 2018.
- **Adjunct Professorship**, Department of Chemistry and Biochemistry, The University of Alabama, Tuscaloosa, AL, U.S.A., October 2018–present.
- **Adjunct Professorship**, Institute for Computational Science (IACS), Stony Brook University, Stony Brook, NY, U.S.A., October 2015–September 2021.
- **Visiting Professorship**, Bremen Center for Computational Material Science (BCCMS), Bremen University, Germany, June-July 2018.
- **Author Profile**, *Angew. Chem. Int. Ed.* **57**, 6732 (2018). 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.
- **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

- **Adjunct Faculty**, The Bredesen Center for Interdisciplinary Research and Graduate Education, The University of Tennessee, Knoxville, TN, U.S.A., May 2019–present.
- **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

The University of Tennessee, Knoxville

- Bredesen Center Adjunct Faculty Member

Nagoya University

- PI and/or Co-PI in Department Level Research Proposals until 2017:
  - 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

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

Citation statistics (ISI Thomson Reuters; May 14, 2019): 6200 total citations, h-factor: 42.
Number of articles (August 20, 2018) in journals with impact factor (IF) > 10:

- Nano Letters (IF=13.592): 3
- ACS Nano (IF=12.881): 6
- The Journal of the American Chemical Society (IF=12.113): 14
- Nature Communications (IF=11.47): 5
- Angewandte Chemie International Edition (IF=11.26): 11

Number of journal cover images: 16.

Original Articles in Peer-Reviewed Journals

2019

1. J. H. Moon, P. Manandhar, M. R. Rohman, L. Mathivathanan, K. H. Lee, S. Irle, Phenyleneethynylene trimer-based rigid-flexible [2+2] macrocycles for nucleic acid labelling in live cells, Chem. Commun., accepted (2019).
2. T. Hayashi, K. H. Lee, H. Iida, E. Yashima, S. Irle, Y. Hijikata, The helix-inversion mechanism in double-stranded helical oligomers bridged by rotary cyclic boronate esters, J. Comp. Chem. accepted (2019). DOI: 10.1002/jcc.25856
3. V. Q. Vuong, Y. Nishimoto, D. G. Fedorov, B. G. Sumpter, T. A. Niehaus, S. Irle, The Fragment Molecular Orbital Method Based on Long-range Corrected Density-Functional Tight-Binding, J. Chem. Theory Comput. Accepted (2019). DOI: 10.1021/acs.jctc.9b00108
4. N. Ousaka, S. Yamamoto, H. Iida, T. Iwata, S. Ito, Y. Hijikata, S. Irle, E. Yashima, Water-mediated deracemization of a bisporphyrin helicate assisted by diastereoselective encapsulation of chiral guests, Nat. Communications accepted 3/6/2019
5. S. Moon, Y. Hijikata, S. Irle, Structural transformations of graphene exposed to nitrogen plasma: quantum chemical molecular dynamics simulations, Phys. Chem. Chem. Phys., Advance Article (2019). DOI: 10.1039/C8CP06159A Featured on Journal Front Cover.

6. C. A. Eveleens, S. Irle, A. J. Page, How does acetonitrile modulate single-walled carbon nanotube diameter during CVD growth? Carbon 146, 535-541 (2019). DOI: 10.1016/j.carbon.2019.02.027

7. R. Kimura, Y. Hijikata, C. A. Eveleens, A. J. Page, S. Irle, Chiral-Selective Etching Effects on Carbon Nanotube Growth at Edge Carbon Atoms, J. Comp. Chem. 40(2), 375-380 (2019). Memorial Festschrift for Keiji Morokuma. DOI: 10.1002/jcc.25610

2018

8. D. Uraguchi, K. Kuwata, Y. Hijikata, R. Yamaguchi, H. Imaizumi, A. M. Sathiyanarayanan, C. Rakers, N. Mori, K. Akiyama, S. Irle, P. McCourt, T. Kinoshita, T. Ooi, Y. Tsuchiya, *A femtomolar-range suicide germination stimulant for the parasitic plant Striga hermonthica,* Science **362**(6420), 1301-1305 (2018). DOI: 10.1126/science.aau5445

9. K. H. Lee, U. Schnupf, B. G. Sumpter, S. Irle, *Performance of Density-Functional Tight-Binding in Comparison to Ab Initio and First-Principles Methods for Isomer Geometries and Energies of Glucose Epimers in Vacuo and Solution,* ACS Omega **3**, 16899-16915 (2018). DOI: 10.1021/acsomega.8b02213

10. Z. Li, N. Huang, K. H. Lee, Y. Feng, S. Tao, Q. Jiang, Y. Nagao, **S. Irle**, D. Jiang, *Light-Emitting Covalent Organic Frameworks: Fluorescence Improving via Pinpoint Surgery and Selective Switch-On Sensing of Anions,* J. Am. Chem. Soc., accepted (2018). DOI: 10.1021/jacs.8b08380

11. C.-P. Chou, H. A. Witek, and **S. Irle**, *When finite becomes infinite: Convergence properties of vibrational spectra of oligomer chains,* J. Mol. Model. accepted (Pratim Chattaraj Festschrift)

12. R. Kimura, Y. Hijikata, C. A. Eveleens, A. J. Page, **S. Irle,** *Chiral-selective Etching Effects on Carbon Nanotube Growth at Edge Carbon Atoms,* J. Comp. Chem. accepted (Morokuma Festschrift) (2018).

13. R. Daengngern, C. Camacho, N. Kungwan, **S. Irle,** *Theoretical prediction and analysis of the UV/Vis absorption and emission spectra of chiral carbon nanorings,* J. Phys. Chem. A, ASAP article (2018). DOI: 10.1021/acs.jpca.8b07270

14. H.-W. Wang, L. Vlcek, J. C. Neuefeind, K. Page, **S. Irle**, J. M. Simonson, A. G. Stack, *Decoding Oxyanion Aqueous Solvation Structure: A Potassium Nitrate Example at Saturation,* J. Phys. Chem. B **122**, 7584-7589 (2018). DOI: 10.1021/acs.jpcb.8b05895

15. I. Mitchell, **S. Irle**, A. J. Page, *Inducing Regioselective Chemical Reactivity in Graphene with Alkali Metal Intercalation,* Phys. Chem. Chem. Phys. **20**, 19987-19994 (2018). DOI: 10.1039/c8cp02903b

16. S. Ito, Y. Wang, Y. Okamoto, **S. Irle**, *Quantum Chemical Replica-Exchange Umbrella Sampling Molecular Dynamics Simulations Reveal the Formation Mechanism of Iron Phthalocyanine from Iron and Phthalonitrile,* J. Chem. Phys. **149**, 072332/1-10 (2018). DOI: 10.1063/1.5026956

17. C. Hanpaibool, T. Chakcharoensapa, Arifin, Y. Hijikata, **S. Irle**, P. Wolschann, N. Kungwan, P. Pongsawasdi, P. Ounjai, T. Rungrotmongkol, *Theoretical analysis of*

orientations and tautomerization of genistein in β-cyclodextrin, J. Mol. Liq. **265**, 16-23 (2018). DOI: 10.1016/j.molliq.2018.05.109

18. F. J. Dominguez-Gutierrez, P. S. Krstic, **S. Irle**, R. Cabrera-Trujillo, *Low-energy hydrogen uptake by small-cage C_n and $C_{n-1}B$ fullerenes,* Carbon **134**, 189-198 (2018). DOI: 10.1016/j.carbon.2018.03.085

19. P. S. Krstic, L. Han, **S. Irle**, H. Nakai, *Quantum classical molecular dynamics simulations and analysis of boron nitride nanostructure plasma synthesis from a hot, high pressure gas,* Chem. Sci. **9**, 3803-3819 (2018). DOI: 10.1039/C8SC00667A

20. S. Ito, D. G. Fedorov, Y. Okamoto, **S. Irle,** *Implementation of replica-exchange umbrella sampling in GAMESS*, Comp. Phys. Commun. **228**, 152-162 (2018). DOI: 10.1016/j.cpc.2018.01.014

21. N. Suzuki, K. Suda, D. Yokogawa, H. Kitoh-Nishioka, **S. Irle**, K. Kamada, A. Fukazawa, S. Yamaguchi, *Near Infrared Two-Photon-Excited and -Emissive Dyes Based on a Strapped Excited-State Intramolecular Proton-Transfer (ESIPT) Scaffold,* Chem. Sci. **9**, 2666-2676 (2018) (Edge Article). DOI: 10.1039/C8SC00066B Featured on Journal Inside Cover.

22. A. Srivastava, T. Hirota, **S. Irle**, F. Tama, *Conformational dynamics of human Protein Kinase CK2α and its effect on function and inhibition,* Proteins: Structure, Function and Bioinformatics **86**(3), 344-353 (2018). DOI: 10.1002/prot.25444

23. V. Q. Vuong, J. A. Kuriappan, M. Kubillus, J. Kranz, T. Mast, T. Niehaus, **S. Irle,** M. Elstner, *Parametrization and Benchmark of LC-DFTB2 for Organic Molecules,* J. Chem. Theory Comput. **14**(1), 115-125 (2018). DOI: 10.1021/acs.jctc.7b00947

24. P. Bhanja, S. K. Das, K. Bhunia, D. Pradhan, T. Hayashi, Y. Hijikata, **S. Irle**, A. Bhaumik, *A new porous polymer for highly efficient capacitive energy storage,* ACS Sustainable Chem. Eng. **6**(1), 202-209 (2018). DOI: 10.1021/acssuschemeng.7b02234

25. S. Mondal, R. Singuru, S. C. Shit, T. Hayashi, **S. Irle**, Y. Hijikata, J. Mondal, A. Bhaumik, *Ru Nanoparticle-Decorated Porous Organic Network for Direct Hydrodeoxygenation of Long Chain Fatty Acids to Alkanes,* ACS Sustainable Chem. Eng. **6**(2) 1610-1619 (2018). DOI: 10.1021/acssuschemeng.7b02772

26. Arifin, D. Yokogawa, U. Schnupf, **S. Irle,** *Statistical Mechanics-Based Theoretical Investigation of Solvation Effects on Glucose Anomer Preferences,* J. Phys. Chem. B, **122**(1) 290-296 (2018). DOI: 10.1021/acs.jpcb.7b10270

2017

27. V. S. Reddy, **S. Irle,** *An indirect intersystem crossing $S_1 \rightarrow T_3/T_2 \rightarrow T_1$ promoted by Jahn-Teller effect in cycloparaphenylenes,* J. Chem. Theory Comput. **13**(10), 4944-4949 (2017). DOI: 10.1021/acs.jctc.7b00166

28. H. Kitoh-Nishioka, K. Welke, Y. Nishimoto, D. G. Fedorov, **S. Irle,** *Multi-Scale Simulations on Charge Transport in Covalent Organic Frameworks: Including Dynamics of Transfer Integrals from FMO-DFTB/LCMO,* J. Phys. Chem. C **121**(33), 17712-17726 (2017). DOI: 10.1021/acs.jpcc.7b05779

29. A. S. Hutama, Y. Hijikata, **S. Irle,** *Coupled Cluster and Density Functional Studies of Atomic Fluorine Chemisorption on Coronene as Model Systems for Graphene Fluorination,* J. Phys. Chem. C, **121**(27), 14888-14898 (2017). DOI: 10.1021/acs.jpcc.7b03627

30. F. J. Dominguez-Gutierrez, F. Bedoya, P. S. Krstic, J. P. Allain, **S. Irle,** C. H. Skinner, R. Kaita, B. Koel, *Unraveling the plasma-material interface with real time diagnosis of dynamic boron conditioning in extreme tokamak plasmas,* Nucl. Fusion **57**(8), 086050/1-7 (2017). DOI: 10.1016/j.nme.2016.11.024

31. L. X. Zhao, Y. Hijikata, **S. Irle**, *Structural Influence of transition metal (Sc, Y, and Lu) atoms inside gold nanoparticles,* Int. J. Quant. Chem. **117**(2), e25371/1-6 (2016). DOI: 10.1002/qua.25371

32. Y. Wang, W. Song, M. Jiao, Z. Wu, **S. Irle,** *Importance of Oxygen in Single-Walled Carbon Nanotube Growth: Insights from QM/MD Simulations,* Carbon **121**, 292-300 (2017). DOI: 10.1016/j.carbon.2017.06.005

33. N. Ozaki, H. Sakamoto, T. Nishihara, T. Fujimori, Y. Hijikata, R. Kimura, **S. Irle**, K. Itami, *Electro-Activated Conductivity and White Light Emission of a Hydrocarbon Nanoring-Iodine Assembly,* Angew. Chem. Int. Ed., Advance Publication, (2017). DOI: 10.1002/anie.201703648 "Hot Paper" of Angew. Chem. Highlighted on Nikkei News http://www.nikkei.com/article/DGXLRSP447431_X00C17A6000000/

34. H.-J. Qian, G. Eres, **S. Irle,** *Quantum Chemical Molecular Dynamics Simulation of Carbon Nanotube-Graphene Welding,* Molecular Simulation **43**(13-16), 1269-1276 (2017) (special issue on the "The 4th International Conference on Molecular Simulation"), DOI: 10.1080/08927022.2017.1328555

35. Y. Wang, H. Jian, Z. Wu, **S. Irle**, *QM/MD Simulations on Graphene Hydrogenation/Deuteration: C_xH/D Formation Mechanism and Isotope Effect,* J. Phys. Chem. C **121**(15), 8480-8489 (2017). DOI: 10.1021/acs.jpcc.7b01662

36. J. Wang, Y.-Y. Zhao, P.-H. Lee, **S. Irle,** *Er^{3+} Photoluminescence in $Er_2@C_{82}$ and $Er_2C_2@C_{82}$ Metallofullerenes Elucidated by Density Functional Theory,* Inorg. Chem. **56**(11), 6576-6583 (2017). DOI: 10.1021/acs.inorgchem.7b00695

37. S. K. Kundu, R. Singuru, T. Hayashi, Y. Hijikata, **S. Irle**, J. Mondal, *Constructing Sulfonic Acid Functionalized Anthracene Derived Conjugated Porous Organic Polymer for Efficient Metal-Free Catalytic Acetalization of Bio-Glycerol,* ChemistrySelect **2**(17), 4705-4716 (2017). DOI: 10.1002/slct.201700901

38. Y. Nishimoto, H. Kondo, K. Yamaguchi, D. Yokogawa, J. Yamaguchi, K. Itami, **S. Irle,** *Theoretical Elucidation of Potential Enantioselectivity in a Pd-Catalyzed Aromatic C-H Coupling Reaction,* J. Org. Chem. Note **82**(9), 4900-4906 (2017). DOI: 10.1021/acs.joc.6b02675

39. T. Fukushima, H. Sakamoto, K. Tanaka, Y. Hijikata, **S. Irle,** K. Itami, *Polymorphism of [6]cycloparaphenylene for packing structure-dependent host-guest interaction,* Chem. Lett. **46**, Advance Publication (2017). DOI: 10.1246/cl.170210 Editor's Choice.

40. Y. Nishimura, T. Tsuneda, T. Sato, M. Katouda, **S. Irle,** *Quantum Chemical Estimation of Acetone Physisorption on Graphene Using Combined Basis Set and Size Extrapolation Schemes,* J. Phys. Chem. C **121**(16), 8999-9010 (2017). DOI: 10.1021/acs.jpcc.6b13002

41. H. Iida, K. Ohmura, R. Noda, S. Iwahana, H. Katagiri, N. Ousaka, T. Hayashi, Y. Hijikata, **S. Irle,** E. Yashima, *Double-Stranded Helical Oligomers Covalently Bridged by Rotary Cyclic Boronate Esters,* Chem. Asian J. **12**, 927-935 (2017). DOI: 10.1002/asia.201700162 Featured on Journal Front Cover, DOI: 10.1002/asia.201700350. Highlighted on ChemistryViews.org

42. H. Kitoh-Nishioka, D. Yokogawa, **S. Irle,** *Förster Resonance Energy Transfer between Fluorescent Proteins: Efficient Transition Charge-Based Study,* J. Phys. Chem. C **121**(8), 4220-4238 (2017). DOI: 10.1021/acs.jpcc.7b00833

43. P. Bhanja, K. Bhunia, S. K. Das, D. Pradhan, R. Kimura, Y. Hijikata, **S. Irle,** A. Bhaumik, *New Triazine Based Covalent Organic Framework for High-Performance Capacitive Energy Storage,* ChemSusChem **10**(5), 921-929 (2017). DOI: 10.1002/cssc.201601571

44. Y. Surakhot, V. Laszlo, C. Chitpakdee, V. Promarak, T. Sudyoadsuk, N. Kungwan, T. Kowalczyk, **S. Irle,** S. Jungsuttiwong, *Theoretical rationalization for reduced charge recombination in bulky carbazole-based sensitizers in solar cells,* J. Comp. Chem. **38**(12), 901-909 (2017). DOI: 10.1002/jcc.24751 Featured on Journal Front Cover, DOI: 10.1002/jcc.24751

45. Y. Hirakawa, H. Shinohara, K. Welke, **S. Irle,** Y. Matsubayashi, K. U. Torii, N. Uchida, *Cryptic bioactivity capacitated by synthetic hybrid plant peptides,* Nature Commun. **8**, 14318/1-7 (2017). DOI: 10.1038/ncomms14318

46. Y. Wang, M. Jiao, Z. Wu, **S. Irle,** *Theoretical Studies on Ethanol Dissociation on Iron Nano-Particles in the Early Stage of SWCNT Growth,* J. Phys. Chem. C **121**(4), 2276-2284 (2017). DOI: 10.1021/acs.jpcc.6b12207

47. Y. Nishimoto, **S. Irle,** *Quantum chemical prediction of vibrational spectra of large molecular systems with radical or metallic electronic structure,* Chem. Phys. Lett. **667**, 317-321 (2017). DOI: 10.1016/j.cplett.2016.11.014 Highlighted on "Advances in Engineering"

2016

48. I. S. Fedorov, A. A. Kuzubov, A. Kholtobina, E. A. Kovaleva, J. Knaup, **S. Irle,** *Theoretical Investigation of Molecular and Electronic Structures of Buckminsterfullerene-Silicon Quantum Dot Systems,* J. Phys. Chem. A **120**, 9767-9775 (2016). DOI: 10.1021/acs.jpca.6b06959

49. R. Nozawa, H. Tanaka, W.-Y. Cha, Y. Hong, I. Hisaki, S. Shimizu, J.-Y. Shin, T. Kowalczyk, **S. Irle**, D. Kim, H. Shinokubo, *Stacked antiaromatic porphyrins,* Nature Commun. **7**, 13620/1-7 (2016). DOI: 10.1038/ncomms13620

50. T. Hayashi, Y. Hijikata, A. J. Page, D. Jiang, **S. Irle,** *Theoretical analysis of structural diversity of covalent organic framework: Stacking isomer structures thermodynamics and kinetics,* Chem. Phys. Lett. **664**, 101-107 (2016). DOI: 10.1016/j.cplett.2016.09.071

51. X. Feng, X. Ding, L. Chen, Y. Wu, L. Liu, M. Addicoat, **S. Irle**, Y. Dong, D. Jiang, *Two-dimensional artificial light-harvesting antennae with predesigned high-order structure and robust photosensitising activity,* Sci. Rep. **6**, 32944/1-13 (2016). Open Access. DOI: 10.1038/srep32944

52. I. A. Eveleens, Y. Hijikata, **S. Irle,** A. J. Page, *Chirality-Selective Carbon Nanotube Etching with Ammonia: A Quantum Chemical Investigation,* J. Phys. Chem. C **120**(35), 19862-19870 (2016). DOI: 10.1021/acs.jpcc.6b06997

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Others

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3. Q. Cui, **S. Irle**, D. Musaev, *Keiji Morokuma (1934-2017) – Inspiring Molecular Quantum Chemist,* Angew. Chem. Int. Ed. Early View (2017). DOI: 10.1002/anie.201800390
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2. FMO-DFTB implementation in GAMESS-US, Y. Nishimoto, D. G. Fedorov, S. Irle, 2014.
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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
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- Environmental Science & Technology
- EPL Journal
- Inorganic Chemistry Frontiers
- International Journal of Chemical Kinetics
- International Journal of Mass Spectroscopy
- Internet Electronic Journal of Molecular Design
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- 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
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- Journal of Physical Chemistry A/B/C

- Journal of Physics and Chemistry of Solids
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- Materials & Design
- Materials Chemistry and Physics
- Materials Science & Engineering C
- Mathematical and Numerical Modeling of Flow and Transport
- Molecular Physics
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- Nano Letters
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- 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.
- American Physical Society, 2017–present.
- The Chemical Society of Japan, 2006–2017.
- 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. April 22–26, 2019: 2019 MRS Spring Meeting and Exhibit, ES05 "Cooperative Catalysis for Energy and Environmental Applications", Phoenix, AZ, U.S.A., **S. Irle**, *"Approximate Density Functional Theory for Heterogeneous Catalysis"*
2. 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"*
3. 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"*
4. 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"*
5. 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)"*
6. 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"*
7. 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"*.
8. December 15–20, 2015: Pacifichem 2015, Honolulu, HI, U.S.A.: **S. Irle**, *"Calculation of Charge Carrier Mobility in Covalent Organic Frameworks"*.
9. 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"*.
10. 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"*.
11. 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"*
12. 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"*
13. 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"*

14. 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"*
15. 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"*
16. 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"*
17. 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"*
18. 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"
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,** *"TD-DFTB/MD Simulation of UV/Vis Fluorescence Spectra"*
20. 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"*
21. November 21, 2013: "International Symposium on Atomic Cluster Catalysis", Tsinghua University, Beijing, China, **S. Irle**, *"Introduction to the density-functional tight-binding (DFTB) method"*
22. 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"*
23. 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"*
24. 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"*

25. 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"*
26. 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"*
27. 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"*
28. 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"*
29. 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"*
30. 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"*
31. 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"*
32. April 12–16, 2013: The Sixth NASA, Air Force Research Laboratory, Honda, and 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"*
33. 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"*
34. 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"*
35. 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"*

36. 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"*
37. 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"*
38. 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"*
39. 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"*
40. March 12–13, 2012: "1st Campus Asia Symposium", Nagoya University, Japan: **S. Irle**, *"Quantum Chemistry of Complex Systems"*
41. 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"*
42. 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"*
43. 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"*
44. 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"*
45. 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"*
46. 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"*
47. 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"*
48. 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"*
49. 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"*

50. October 14, 2010: DFTB summer school workshop at Kasetsart University, Bangkok, Thailand: **S. Irle**, *"Quantum chemical molecular dynamics simulations of combustion fullerene synthesis",*
51. 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"*
52. 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"*
53. 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".*
54. 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"*
55. 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"*
56. 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*"
57. 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"*
58. 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".*
59. 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"*
60. 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

1. 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"*
2. 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"*
3. 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"*
4. 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)"*
5. 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"*
6. September 1–4, 2010: GCOE meeting of the Department of Chemistry, Tohoku University, Sendai: *"Graphene: molecular structure, vibrational spectroscopy, and hydrogen chemisorption"*
7. August 9, 2010: IMS Okazaki: **S. Irle,** *"Current state and future directions of quantum chemical MD simulations"*
8. July 9, 2010: IMS Okazaki: **S. Irle,** *"Bears, Bubbles, and Hot Carbon"*
9. October 3–4, 2008: 2008, Hazu Onsen: **S. Irle,** *"Recent progress in quantum chemical molecular dynamics simulations of giant metallofullerene formation"*

10. 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.

Jun 25, 2018 — Seminar Talk, Bremen Center for Computational Sciences, Bremen University, Bremen, Germany: **S. Irle**, *"Opportunities for chemical sciences-driven expansion of the DFTB method at the Oak Ridge National Laboratory"*

Feb 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"*

Jan 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"*

Oct 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"*

Oct 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"*

Sep 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"*

Feb 15, 2017 — Department of Chemistry, Costa Rica University, San Jose, Costa Rica: **S. Irle,** *"Quantum Chemical Method for the Study of Complex Systems"*

Aug 18, 2016 — Bremen Center for Computational Material Sciences (BMCS), University of Bremen, Germany: **S. Irle,** *"Towards quantum chemical molecular dynamics simulations of soft materials"*

Jul 7, 2016 Seminar at the Department of Chemistry, Siberian Federal University, Krasnoyarsk, Russia: **S. Irle,** *"The Power of Molecules – The Power of Computation"*

Jun 20-21, 2016 *"FMO-DFTB Mini-Workshop",* Nagoya University, Japan: **S. Irle,** *"Approximate DFT Methods for Extended Systems"*

Apr 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"*

Apr 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"*

Apr 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"*

Apr 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"*

Dec 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"*

Nov 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).

Nov 19, 2014 Department Seminar, Department of Chemistry, Hokkaido University, Sapporo, Japan: **S. Irle,** *"Recent methodological developments for the quantum chemical study of complex systems"*

Sep 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"*

Jun 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"*

Jun 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"*

Apr 15, 2014 Seminar at DENSO Company, Nisshin City, Japan: **S. Irle,** *"How quantum chemistry can help industry R&D"*

Feb 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"*

Sep 27, 2013 Department Seminar at the School of Engineering and Science, Jacobs University, Bremen, Germany: **S. Irle,** *"Excited States of Large Molecules"*

Apr 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"*

Dec 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

Dec 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?"*

Nov 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?"*

Oct 24, 2012 Japan Fine Ceramics Center, Nagoya, Japan: **S. Irle,** *"Mechanism of carbon nanotube and graphene formation during high-temperature vacuum decomposition of SiC"*

Oct 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"*

Sep 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"*

Apr 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"*

Mar 6, 2012 "GCOE Delegates Meeting for Participants from Malaysia and Indonesia", Nagoya University, Japan: **S. Irle**, *"Quantum Chemistry of Complex Systems"*

Feb 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"*

Feb 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"*

Feb 13, 2012 Department of Chemistry Seminar, Yokohama City University, Yokohama, Japan: **S. Irle,** *"Quantum chemical molecular dynamics simulations of graphene hydrogenation"*

Dec 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"*

Oct 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"*

Oct 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"*

Oct 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"*

Jul 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)

Mar 15, 2011 Seminar at the Department of Chemistry, Siberian Federal University, Krasnoyarsk, Russia: invited: *"DFT-based simulations of thermally and optically excited nanomaterials"*

Mar 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"*

Jan 27, 2011 Nanosystem Research Institute, AIST, Tsukuba, Japan, *"Density-Functional Tight-Binding: Theory and Recent Developments"*

Jan 26, 2011 Nanotube Research Center, AIST, Tsukuba, Japan, *"New quantum chemical MD simulations of nanocarbon structure formation"*

Dec 2, 2010 Department of Physics, Göteborg University, Sweden, **S. Irle,** *"Fullerenes, nanotubes, graphenes: insights for synthesis from theory"*

Jun 14, 2010 Department of Chemistry, Tohoku University, Sendai, Japan, **S. Irle**, *"Laser heating, collisions, and coalescence of functionalized fullerenes"*

Jun 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"*

Jun 7, 2010 L. Kirensky Institute of Physics, Russian Academy of Sciences, Krasnoyarsk, **S. Irle,** *"Graphene: molecular structure, vibrational spectroscopy, and hydrogen adsorption"*

Apr 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"*

Apr 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"*

Apr 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"*

Apr 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"*

Mar 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"*

Mar 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"*

Dec 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"*

Dec 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"*

Nov 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"*

Nov 24, 2009 Global MBA Program, National Chiao Tung University, Hsinchu, Taiwan: invited: *"Globalization from a Science and Technology Perspective"*

Nov 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"*

Sep 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"*

Sep 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"*

Jul 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"*

Jun 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"*

Jun 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"*

Apr 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,

Feb 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"*

Jan 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"*

Jan 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"*

Jan 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"*

Nov 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"*

Nov 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"*

Jul 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"*

Jun 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"*

Mar 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"*

Mar 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"*

Mar 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"*

Feb 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"*

Oct 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"*

Aug 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"*

Apr 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"

Apr 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"*

Jan 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"*

Jan 2007 — Department of Physics, Kyoto University, Kyoto, Japan: *"Quantum Chemical Molecular Dynamics Simulations of Fullerene and Carbon Nanotube Self-Assembly"*

Aug 2006 — Nagoya University and Japan Fine Ceramics Center, Nagoya, Japan: *"Quantum Chemical Molecular Dynamics Simulations of Metallofullerene Formation and Carbon Nanotube Nucleation Processes"*

Aug 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"*

Apr 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"*

Oct 2005 — Japan Fine Ceramics Center, Nagoya: *"Theory and Experiment Agree: SWNT Caps Grow Catalyst Free with Chirality Preference on SiC Surfaces"*

Oct-Nov 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"*

Sep 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"*

Aug 2004	Nagoya University, Nagoya, Japan: *"Order Out of Chaos: Computer Simulations of High-T Carbon"*
Jul 2004	University of Paderborn, Germany: *"Applications of ONIOM in nanotechnology with emphasis on the DFTB method"*
Jun 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"*
Apr 2002	University of Puerto Rico, San Juan, U.S.A.: "*New technical evolution of the ONIOM method and applications to problems in nanotechnology*"
Sep 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"*
Apr 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"*
Oct 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 2014–2015	Undergraduate Course "Quantum Chemistry III" for junior level students in English, Nagoya University, Japan. Part of the Nagoya University G30 program.
Fall semester 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 2007–2014	Graduate Course "Advanced Quantum Chemistry: Molecular Dynamics Simulations in Highly Reactive Environments", Department of Chemistry, University of Nagoya, Japan.
Summer semester 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 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, 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)

Winter 2016–Winter 2017 Dr. Christin Rakers, PhD: Humboldt University, Germany. Research topic: "Studies of Striga suicide germination mechanisms". Present position: Junior Associate Professor, Graduate School and Faculty of Pharmaceutical Sciences, Kyoto University.

Spring 2016–Summer 2017 Dr. Shingo Ito, PhD: Nagoya University. Research topic: "Replica exchange MD simulations with DFTB". 3 papers published. Present position: Postdoc, Boston University.

Fall 2016–Spring 2017 Dr. Supriya Saha, PhD: Visva-Bharati University, India. Research topic: "DFTB parameterization of metal alloys in combination with CHON elements". Present position: Scientist, Chemical Sciences and Technology Division, CSIR-NEIST, Jorhat, Assam, India.

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". 1 paper published. Present position: Associate Professor, East China University of Science and Technology, Shanghai, China.

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. 3 papers published. Present position: Schrodinger, Inc., Mannheim, Germany.

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.

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.

Spring–Fall 2015 Dr. Arthithaya Meeprasert, PhD: Chulalongkorn University. Visiting from Chulalongkorn University. Research topics: Classical biosimulations, QM/MM simulations.

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.
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.
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.
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.
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.
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: Junior Lecturer, Department of Chemistry, Unviersity of Nottingham-Trent, England.
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.
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.
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.
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.
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

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

Co-supervised with Prof. Keiji Morokuma, Emory University

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

GRADUATE STUDENTS SUPERVISED (10 MEMBERS OF MY GROUP, 31 VISITING OR CO-SUPERVISED)

Fall 2018	Junmian Zhu, visiting from Department of Chemistry, University of Madison-Wisconsin, ORSS student.
Fall 2016–present	Ka Hung Lee, Department of Chemistry, Nagoya University, since 2017: Bredesen Center, University of Tennessee Knoxville, U.S.A.
Fall 2016–present	Quan V. Vuong, Department of Chemistry, Nagoya University, since 2017: Bredesen Center, University of Tennessee Knoxville, U.S.A.

Fall 2015–Spring 2018	Longtao Han, Institute of Advanced Computational Sciences, Stony Brook University, U.S.A.
Spring 2014–present	Mr. Taku Hayashi, Department of Chemistry, Nagoya University, Japan.
Fall 2013–Fall 2017	Mr. Aulia Sukma Hutama, Institute of Technology, Bandung, Indonesia (G30 fellow)
Fall 2012–Fall 2016	Mr. Arifin, Institute of Technology, Bandung, Indonesia (G30 fellow)
Spring 2012–Spring 2016	Dr. Kosuke Usui, Department of Chemistry, Nagoya University (present position: Kobayashi Pharmaceutical Co., Ltd., Osaka, Japan).
Fall 2015	Mr. Junda Li, visiting from Department of Chemistry, University of Adelaide, Australia.
Spring–Fall 2015	Mr. Chanchai Sattayanon, visiting from Chiang Mai University, Thailand.
Spring–Summer 2015	Mr. Mathias Piescheck, visiting from the Braunschweig University of Technology, Germany.
Spring–Summer 2015	Mr. Izaac Mitchel, visiting from The University of Newcastle, Australia.
Spring–Winter 2015	Ms. Jenny Pirello, visiting from the University of Calabria, Italy
Fall 2014–Fall 2015	Mr. Rathawat Daengngern, visiting from Chiang Mai University, Thailand.
Spring 2013–Spring 2015	Mr. Naoto Baba, Department of Chemistry, Nagoya University
Fall 2014–Spring 2015	Mr. Ruangchai Tarsang, visiting from Ubon Ratchathani University, Thailand.
Fall 2014–Spring 2015	Ms. Evgeniia Kovaleva, visiting from Siberian Federal University, Krasnoyarsk, Russia.
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)
Spring–Fall 2014	Mr. Pharit Kamsri, visiting from Ubon Ratchathani University, Thailand.
Fall 2013–Spring 2014	Mr. Qingming Deng, visiting from Leibniz Institute for Solid State and Materials Research (IFW), Germany.
Spring–Summer 2013	Ms. Yaowarat Surakhot, visiting from Ubon Ratchathani University, Thailand.
Spring–Summer 2013	Mr. Rathawat Daengngern, visiting from Chiang Mai University, Thailand.

Spring–Fall 2012	Ms. Chonpoonut Rungnim, visiting from Department of Chemistry Chulalongkorn University, Bangkok, Thailand.
Spring 2010–Spring 2013	Mr. Noriyuki Ogasawara (co-supervision with Prof. Michiko Kusunoki), Ecotopia, Nagoya University
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)
Spring 2009–Spring 2012	Dr. Kazuhiko Nagura (co-supervision with Prof. Shigehiro Yamaguchi), Department of Chemistry, Nagoya University
Fall 2008–Spring 2012	Dr. Lili Liu, Department of Chemistry, Nagoya University (present position: postdoctoral fellow in Beijing, China)
Spring 2008–Spring 2013	Dr. Yoshifumi Nishimura, Department of Chemistry, Nagoya University (present position: postdoctoral fellow at Waseda University, Japan)
Spring–Summer 2011	Ms. Elena A. Vishnyakova, visiting from Siberian Federal University, Krasnoyarsk, Russia
Spring 2011	Mr. Danny Haberer, visiting from the University of Vienna, Austria.
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)
Spring 2009–Spring 2011	Mr. Masato Morita (co-supervision with Prof. Michiko Kusunoki), Ecotopia, Nagoya University (present position: Chemical Industry, Japan)
Spring 2009–Spring 2011	Mr. Hironori Hara, Department of Chemistry, Nagoya University (present position: Transportation Industry, Shizuoka)
Summer 2010	Dr. Chatchawal Wongchoosuk, visiting from Mahidol University, Bangkok, Thailand (JENESYS participant) (present position: lecturer, Mahidol University, Bangkok, Thailand)
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)
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)
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

Fall 2003–2007	Dr. Zhi Wang (co-supervision with Prof. Keiji Morokuma), Department of Chemistry, Emory University (present position: banking industry, Hong Kong)
Fall 2001–Summer 2006	Dr. Guishan Zheng (co-supervision with Prof. Keiji Morokuma), Department of Chemistry, Emory University (present position: banking industry).
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).

UNDERGRADUATE STUDENTS SUPERVISED (26 MEMBERS OF MY GROUP, 13 VISITING OR CO-SUPERVISED)

Summer 2018	Mr. Mouhmad H. Elyyan, visiting from Department of Chemical Engineering, Tennessee Technology University, SULI student
Fall 2016–Spring 2017	Mr. Ryosuke Shimizu, Department of Chemistry, Nagoya University
Spring 2016–Spring 2017	Mr. Ryuto Kimura, Department of Chemistry, Nagoya University
Spring 2016–Spring 2017	Mr. Shouta Nakataki, Department of Chemistry, Nagoya University
Spring 2016–Spring 2017	Mr. Naoto Inai, Department of Chemistry, Nagoya University
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.
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.
Spring 2015–Spring 2016	Mr. Katsuhiro Ito, Department of Chemistry, Nagoya University
Spring 2015–Spring 2016	Mr. Naohiro Obata, Department of Chemistry, Nagoya University (present position: Resorttrust, Nagoya, Japan).
Summer 2015	Ms. Chonnikan “Kungking” Hanpaibool, Department of Chemistry, Nagoya University, visiting from Mahidol University, Bangkok, Thailand
Fall 2014–Fall 2015	Ms. Raashida Tan, Department of Chemistry, Nagoya University, G30 program.
Spring 2014–Spring 2015	Mr. Yasumasa Namba, Department of Chemistry, Nagoya University
Spring 2014–Spring 2015	Mr. Mikinori Ando, Department of Chemistry, Nagoya University
Spring 2014–Spring 2015	Mr. Ryotaro Yamada, Department of Chemistry, Nagoya University
Spring 2013–Spring 2014	Mr. Yuya Akao, Department of Chemistry, Nagoya University

Spring 2013–Spring 2014	Mr. Masachika Kato, Department of Chemistry, Nagoya University
Spring 2013–Spring 2014	Ms. Mari Shibata, Department of Chemistry, Nagoya University
Spring 2012–Spring 2013	Mr. Naoto Baba, Department of Chemistry, Nagoya University
Spring 2012–Spring 2013	Mr. Jun Kato, Department of Chemistry, Nagoya University
Spring 2011–Spring 2012	Mr. Shinsuke Iwata, Department of Chemistry, Nagoya University
Spring 2011–Spring 2012	Ms. Ayaka Ban, Department of Chemistry, Nagoya University
Spring 2011–Spring 2012	Mr. Syou Fukuoka, Department of Chemistry, Nagoya University
Spring 2010–Spring 2011	Mr. Ryota Umeda, Department of Chemistry, Nagoya University
Spring 2010–Spring 2011	Mr. Kousuke Usui, Department of Chemistry, Nagoya University
Spring 2010–Spring 2011	Mr. Yoshitaka Okita, Department of Chemistry, Nagoya University
Spring 2009–Spring 2010	Mr. Yoshio Kato, Department of Chemistry, Nagoya University
Spring 2009–Spring 2010	Mr. Yoshio Nishimoto, Department of Chemistry, Nagoya University
Spring 2009–Spring 2010	Mr. Takahisa Fujimori, Department of Chemistry, Nagoya University
Spring 2008–Spring 2009	Mr. Hironori Hara, Department of Chemistry, Nagoya University
Spring 2008–Spring 2009	Mr. Kazuhiko Nagura (co-supervised with Prof. Shigehiro Yamaguchi), Department of Chemistry, Nagoya University
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
Fall 2007–Spring 2012	Mr. Sho Shindo (co-supervised with Prof. Keiji Morokuma), Fukui Institute for Fundamental Chemistry, Kyoto University
Spring 2007–Spring 2008	Mr. Yoshifumi Nishimura, Department of Chemistry, Nagoya University
Fall 2006–Spring 2008	Mr. Daiki Ishida (co-supervised with Prof. Keiji Morokuma), Fukui Institute for Fundamental Chemistry, Kyoto University
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
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
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

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
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

10 MOST SIGNIFICANT PUBLICATIONS

1. R. Nozawa, H. Tanaka, W.-Y. Cha, Y. Hong, I. Hisaki, S. Shimizu, J.-Y. Shin, T. Kowalczyk, **S. Irle**, D. Kim, H. Shinokubo, Stacked antiaromatic porphyrins, *Nature Commun.* **7**, 13620/1-7 (2016). http://dx.doi.org/10.1038/ncomms13620
2. H. Nishizawa, Y. Nishimura, M. Kobayashi, **S. Irle,** H. Nakai, Three pillars for achieving quantum mechanical molecular dynamics simulations of huge systems: divide-and-conquer, density-functional tight-binding, and massively parallel computation, *J. Comp. Chem.* **37**(21), 1983-1992 (2016). http://dx.doi.org/10.1002/jcc.24419
3. Y. Nishimoto, D. G. Fedorov, **S. Irle,** Density-functional tight-binding combined with the fragment molecular orbital method, *J. Chem. Theory Comput.* **10**(11), 4801–4812 (2014). http://dx.doi.org/10.1021/ct500489d [featured on journal's cover; highlighted Dec. 4–15, 2014, as "Ultrafast complex molecular simulations by 'cutting up molecules'" in various online science news websites, see http://www.itbm.nagoya-u.ac.jp/en/research/2014/12/Irle-FMO-DFTB.php]
4. J. Guo, Y. Xu, S. Jin, L. Chen, T. Kaji, Y. Honsho, M. A. Addicoat, J. Kim, A. Saeki, H. Ihee, S. Seki, **S. Irle**, M. Hiramoto, J. Gao, D. Jiang, Conjugated organic framework with three-dimensionally ordered stable structure and delocalized π clouds, *Nature Commun.* **4**, 2736 (2013). http://dx.doi.org/10.1038/ncomms3736 [highlighted in *Synfacts* **10**(2), 0147 (2014), http://dx.doi.org/10.1055/s-0033-1340605]
5. H. Wang, S. Hamanaka, Y. Nishimoto, **S. Irle,** T. Yokoyama, H. Yoshikawa, K. Awaga, In operando X-ray absorption fine structure studies of polyoxometalate molecular cluster batteries: polyoxometalates as electron sponges, *J. Am. Chem. Soc.* **134**, 4918-4924 (2012). http://dx.doi.org/10.1021/ja2117206 [highlighted in *ChemInform* **43**, 2012, http://dx.doi.org/10.1002/chin.201227011]
6. X. Feng, L. Liu, Y. Honsho, A. Saeki, S. Seki, **S. Irle**, Y. Dong, A. Nagai, D. Jiang, High-rate charge-carrier transport in porphyrin covalent organic frameworks: switching from hole to electron to ambipolar conduction, *Angew. Chem. Int. Ed.* **124**(11), 2672-2676 (2012). http://dx.doi.org/10.1002/ange.201106203
7. X. Ding, L. Chen, Y. Honsho, X. Feng, O. Saengsawang, J. Guo, A. Saeki, S. Seki, **S. Irle,** S. Nagase, V. Parasuk, and D. Jiang, An *n*-channel two-dimensional covalent organic framework, *J. Am. Chem. Soc.* (Communication) **133**, 14510-14513 (2011). http://dx.doi.org/10.1021/ja2052396 [highlighted in *C&E News* **89** (37), 21 (2011)].
8. G. Zheng, H. A. Witek, P. Bobadova-Parvanova, **S. Irle,** D. G. Musaev, R. Prabhakar, K. Morokuma, M. Lundberg, M. Elstner, Ch. Köhler, Th. Frauenheim, Parameter calibration of transition-metal elements for the spin-polarized self-consistent-charge density-functional tight-binding (DFTB) method: Sc, Ti, Fe, Co, and Ni, *J. Chem. Theory Comput.* **3**(4), 1349-1367 (2007). http://dx.doi.org/10.1021/ct600312f
9. **S. Irle**, G. Zheng, Z. Wang, K. Morokuma, The C_{60} formation puzzle "solved": QM/MD simulations reveal the shrinking hot giant road of the dynamic fullerene self-assembly mechanism, *J. Phys. Chem. B* **110**(30), 14531-14545 (2006).

http://dx.doi.org/10.1021/jp061173z [feature article; also highlighted in Philip Ball, C_{60}: some assembly required, *Nature Materials Science and Nanotechnology Nanozone*, August 10, 2006].

10. X. Feng, **S. Irle**, H. Witek, K. Morokuma, R. Vidic, E. Borguet, Sensitivity of ammonia interaction with single-walled carbon nanotube bundles to the presence of defect sites and functionalities, *J. Am. Chem. Soc.* **127**(30), 10533-10538 (2005). http://dx.doi.org/10.1021/ja042998u [highlighted in *C&E News* 83, 24 (2005)].