

BRIEF CURRICULUM VITAE

Stephan Irle

Group Leader, Computational Chemistry and Nanomaterials Sciences Group
Computational Sciences and Engineering Division
Computing and Computational Sciences Directorate
Oak Ridge National Laboratory
<https://www.ornl.gov/staff-profile/stephan-irle>
E-mail: irles@ornl.gov



Education

B.S. in Chemistry, University of Siegen, Germany, 1990
M.S. in Chemistry, University of Siegen, Germany, 1992
Ph.D. in Chemistry, University of Vienna, Austria, 1997

Appointments

2020–present: Group Leader, Oak Ridge National Laboratory
2017–present: Senior R&D Staff, Oak Ridge National Laboratory
2019–present: Adjunct Faculty, Bredesen Center, The University of Tennessee, Knoxville
2018–present: Adjunct Faculty, Department of Chemistry & Biochemistry, University of Alabama
2015–present: Adjunct Faculty, Institute of Advanced Computational Science, Stony Brook University
2011–2017: Professor, Department of Chemistry, Nagoya University, Japan
2006–2011: Associate Professor, Department of Chemistry, Nagoya University, Japan
1998–2006: Associate Scientist, Emerson Center, Emory University
1997–1998: Postdoctoral Researcher, Department of Chemistry, Emory University

Research Interests and Expertise

- Advanced atomic-scale simulations of complex systems through approximate quantum chemical methods in combination with machine learning on exascale and quantum computing platforms.
- Applications to driven reactive systems, e.g.: nanostructure formation, heterogeneous catalysis, mineral nucleation and growth in aqueous ionic solutions, ion transport in confined nanomaterials.
- Artificial intelligence solutions for inverse design problems in the chemical and materials sciences.

Scientific Publications

More than 310 publications in peer-reviewed journals, 40 book chapters and conference proceedings, 2 books, 9,300+ citations, h-index: 56. ResearcherID: E-8984-2011, ORCID: 0000-0003-4995-4991.

10 Most Significant Publications

1. Vuong, V. Q.; Madrideo, J. M. L.; Aradi, B.; Sumpter, B. G.; Metha, G. F.; Irle, S. Density-Functional Tight-Binding for Phosphine-Stabilized Nanoscale Gold Clusters, *Chem. Sci.* **2020**, *11*, 13113–13128.
2. Jiang, D.; Huang, N.; Lee, K. H.; Irle, S.; Jiang, Q.; Yue, Y.; Xu, X. A Stable and Conductive Metallophthalocyanine Framework for Electrocatalytic Carbon Dioxide Reduction in Water, *Angew. Chem. Int. Ed.* **2020**, *59*, 16587–16593.
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.* **2019**, *15*(5), 3008–3020.
4. Zhu, J.; Vuong, V. Q.; Sumpter, B. G.; Irle, S. Artificial Neural Network Correction for Density-Functional Tight-Binding Molecular Dynamics Simulations, *MRS Commun.* **2019**, *9*, 867-873.
5. D. Uraguchi, K. Kuwata, Y. Hijikata, R. Yamaguchi, H. Imaizumi, A. M. Sathyanarayanan, C. Rakers, N. Mori, K. Akiyama, S. Irle, P. McCourt, T. Kinoshita, T. Ooi, Y. Tsuchiya, A femtomolar-range suicide germination stimulant for
6. 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**, 1983-1992 (2016).
7. Y. Nishimoto, D. G. Fedorov, S. Irle, *Density-functional tight-binding combined with the fragment molecular orbital method*, *J. Chem. Theory Comput.* **10**, 4801–4812 (2014).
8. 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).

9. 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).
10. S. Irle, G. Zheng, Z. Wang, K. Morokuma, *The C₆₀ formation puzzle "solved": QM/MD simulations reveal the shrinking hot giant road of the dynamic fullerene self-assembly mechanism*, *J. Phys. Chem. B* **110**, 14531-14545 (2006).

Synergistic Activities

1. **Fellow**, American Association for the Advancement of Science (AAAS), since October 2018.
2. **Member**, DOE's National Virtual Biotechnology Laboratory (NVBL) since May 2020, <https://science.osti.gov/nvbl>
3. **Member**, ACS, APS, MRS, Bunsengesellschaft für Physikalische Chemie.
4. **Invited member, IAEA coordinated research project (CRP)** "Erosion and Tritium Retention for Plasma Interaction with Beryllium Surfaces", IAEA, Vienna, Austria, 2012–2016.
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.

Collaborators and Co-editors: B. Aradi (Bremen U.), K. Awaga (Nagoya U.), J. Baudrey (U. Alabama), Q. Cui (Boston U.), P. T. Cummings (Vanderbilt U.), D. A. Dixon (U. Alabama), M. Elstner (Karlsruhe Inst. Technol.), D. G. Fedorov (AIST), T. Frauenheim (Bremen U.), Y. Gotosi (Drexel U.), K. Itami (Nagoya U.), D.-e. Jiang (Riverside U.), D. Jiang (Natl. U. Singapore), F. Lightstone (LLNL), P. S. Krstic (Stony Brook U.), G. Metha (Adelaide U.), H. Nakai (Waseda U.), T. Niehaus (U. Lyon), A. M. N. Niklasson (LANL), Y. Okamoto (Nagoya U.), A. J. Page (U. New Castle), H. Shinohara (Nagoya U.), J. C. Smith (U. Tennessee), F. Tama (Nagoya U.), A. v. Duin (Penn State U.), H. A. Witek (National Chiao Tung U.), S. Yamaguchi (Nagoya U.), E. Yashima (Nagoya U.)

Graduate and Postdoctoral Advisors and Advisees:

Graduate Advisor: H. Lischka (Texas Technol. U.);

Postdoctoral Advisor: K. Morokuma (Emory U.; deceased);

Graduate Students Advised: Arifin (JSR Corporation), Naoto Baba (Nagoya Highschool), Hironori Hara (private company), L. Liu (unknown), Yoshio Nishimoto (Kyoto U.), Yoshifumi Nishimura (Waseda U.), Kosuke Usui (Kobayashi Chemicals), Aulia S. Hutama (Gadjah Mada U.), Taku Hayashi (private company), Quan V. Vuong (Boston U.), Tyler Walker (U. Tennessee, current); **Postdoctoral Scholars Advised:** Matthew A. Addicoat (U. Nottingham-Trent), Cristopher Camacho (U. Costa Rica), Li-Xia Chiao (East China U. Sci. & Technol.), Y. Hijikata (Sapporo U), Shingo Ito (RIKEN), Gang Seob Jung (current), Rabi Khanal (Tokyo Electron Ltd), Hirotaka Kitoh-Nishioka (Kobe U.), Tim Kowalczyk (Western Washington U.), Gabriele Manca (U. Pisa), Arthithaya Meeprasert (Chulalongkorn U.), Christin Rakers (Kyoto U.), Hu-Jun Qian (Jilin U.), Auradee Punkvang (Nakhon Phanom U.), V. Sivaranjana Reddy (U. Hyderabad), Orphan Saengsawang (private industry), Supriya Saha (U. South Carolina), Wichien Sang-aaroon (Rajamangala U. Technol. Isan), Kai Welke (Schrodinger, Inc.), Jian Wang (Hong Kong Polytechnic U.), Ying Wang (Chinese Academy of Sci.), D. Yokogawa (U. Tokyo), Pilsun Yoo (current)

Total number of Graduate Students: 11

Total number of Postdoctoral Scholars: 23