

Curriculum Vitae

Sabre Kais

Goodnight Distinguished Chair in Quantum Computing
Professor, Electrical and Computer Engineering,
Department of Chemistry and Department of Physics
North Carolina State University
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Education

Ph.D., Theoretical Chemistry, Hebrew University of Jerusalem (1989)

Advisors: Prof. R.D. Levine, Prof. M. Cohen

Dissertation: *An Algebraic Approach to Calculate Atomic and Molecular Properties*

M.Sc., Theoretical Chemistry, Hebrew University of Jerusalem (1984)

Thesis: *Atoms in Strong Magnetic Fields: Perturbation Theory Approach*

B.Sc., Chemistry, Hebrew University of Jerusalem (1983)

Academic and Professional Appointments

North Carolina State University

2024–Present — Goodnight Distinguished Chair in Quantum Computing, Electrical and Computer Engineering

2024–Present — Professor, Associate Faculty, Chemistry

2024–Present — Adjunct Professor of Physics

Purdue University

2022–2024 — Director, Center for Quantum Technology (CQT)

2021–2024 — Distinguished Professor of Chemistry

2002–2024 — Professor of Chemical Physics

2023–2024 — Professor, Electrical and Computer Engineering

2010–2024 — Courtesy Professor of Physics

2005–2024 — Courtesy Professor of Computer Science

2021–2023 — Courtesy Professor of Electrical and Computer Engineering

1999–2002 — Associate Professor, Chemistry

1994–1999 — Assistant Professor, Chemistry

Other Research & Visiting Positions

2014–2019 — External Research Professor, Santa Fe Institute
2013–2016 — Research Director, Theory Group, QEERI (Qatar)
2010–2013 — Director, NSF Center for Chemical Innovation
2009 — Visiting Professor, Hebrew University
2010 — Visiting Professor, Technion
2009 — Visiting Professor, King Saud University
2008 — Visiting Scientist, Max Planck Institute (Dresden)
2005 — Guggenheim Fellow, Stanford University
1992 — Visiting Scientist, Cambridge University & Oxford University
1989 — Postdoctoral Associate, Harvard University (D.R. Herschbach, Nobel Laureate 1986)

Honors and Awards

2024 — Miller Visiting Professorship, UC Berkeley
2024 — Graduate Faculty Membership, Physics, NC State
2024 — Goodnight Distinguished Chair in Quantum Computing, NC State
2022 — CMOA Senior Medal, International Workshop on Quantum Systems
2021 — Distinguished Professor of Chemistry, Purdue
2019 — Herbert Newby McCoy Award (Purdue's highest science honor)
2012 — Sigma Xi Research Award
2007 — Fellow, AAAS
2006 — Fellow, American Physical Society
2005 — Guggenheim Fellowship
2004–2009 — Purdue Faculty Scholar
2000 — Forchheimer Fellowship
1998 — NSF CAREER Award
1985 — Landau Prize
1983 — Farkash Prize

Professional Service

Editorial Boards

- Molecular Physics
- Interdisciplinary Sciences: Computational Life Sciences
- Papers in Physics
- Frontiers in Chemistry and Physics
- Scientific Reports
- Quantum Ecosystems Technology Council of India (QETCI)
- Aiscia Informatics (HBKU-Qatar)

Referee and Reviewer

Nature, PRL, PRA/B/E, JCP, PCCP, Nature Communications, NSF, DOE, ARO, ACS PRF, Qatar Foundation, King Fahd University of Petroleum & Minerals (KFUPM), and others.

Organizer and Chair , Conferences, Workshops, and Symposia

- **Organizer and Chair**, Workshop on Quantum Machine Learning for Complex Science and Engineering Problems, North Carolina State University , **June 1 – June 5, 2026**
- **Organizer and Chair** , ADVANCES IN QUANTUM TECHNOLOGIES – ADDRESSING REAL-WORLD CHALLENGES, TechConnect World Innovation Conference, Raleigh , **March 10-12, USA**
- **Organizer and Chair**, Inaugural Industry Advisory Board Meeting, NSF-IUCRC Center for Quantum Technologies, Purdue University, **February 16, 2023**
- **Organizer**, Planning Meeting, Center for Quantum Technologies, Purdue University, **September 30–October 1, 2021**
- **Organizer**, *Quantum Machine Learning and Data Analytics Workshop*, Purdue University, **September 5–6, 2019**
- **Organizer**, ACS Symposium honoring Levine's 80th Birthday, Boston , **August 19, 2018**
- **Organizer & Chair**, Invited Session: *Near-Term Applications of Small-Scale Quantum Computing*, APS March Meeting, **2017**
- **Organizer**, QEERI International Computational Workshop on Solar Energy, **April 2015**
- **Organizer**, 7th Winter School on Quantum Information Science, National Cheng Kung University, **February 2013**
- **Tutorial Organizer & Instructor**, *Quantum Information and Computation for Quantum Chemistry*, APS March Meeting, **March 2013**
- **Organizer**, Banff Workshop on Quantum Information for Quantum Chemistry, Banff, Canada, **June 2011**
- **Organizer**, Winter School in Quantum Information for Quantum Chemistry, Indian Wells, CA, **January 2012**
- **Chair**, Midwest Theoretical Chemistry Conference, Purdue University, **2010**
- **Chair**, Midwest Theoretical Chemistry Conference, Purdue University, 1998
- **Session Chair**, Conductance in Molecules, Fritz Haber Center, Hebrew University, **June 11, 2007**
- **Session Chair**, Electron Dynamics, *The Quantum World in Real Time: Is it Accessible?* Safed , **June 25, 2007**
- **Chair**, Plenary Session on Multi-Scale Simulations, Sanibel Workshop , **2002**

Professional Memberships

- American Chemical Society
- American Physical Society

- AAAS
- Sigma Xi

Personnel

Current Graduate Students

- **Muhammad Arsalan Ali Akbar** (2024–Present), Chemistry — Chirality on quantum computers
- **Nickolas Terehoff** (2025–Present), Physics — Entanglement and chaos in complex Systems
- **Adnan Abulfattah Adnan Jaljuli** (2025–Present) Computer Science — Hybrid HPC and quantum computer
- **Shah Ishmam Mohtashim** (2024–Present), Chemistry — Quantum chemical reactions on quantum computers
- **Turbasu Chatterjee** (2025–Present), ECE, NC State — Quantum machine learning
- **Murat Isik** (2024–Present), ECE, Purdue — Quantum machine learning for health
- **Christian Thrasher** (2024–Present), Physics, NC State — Quantum algorithms
- **Myeongsu Kim** (2023–Present), Computer Science — Quantum machine learning
- **Vinit Kumar Singh** (2021–Present), Chemistry — Quantum computing algorithms
- **Ethan Dickey** (2021–Present), Computer Science — Complexity theory
- **Saurabh Shivpuje** (2021–Present), Chemistry — Quantum computing algorithms

Former Graduate Students

- **Blake Wilson** (2020–2023), ECE — Quantum machine learning
- **Bilal Khalid** (2020–2024), Physics — Quantum topological phase transitions
- **Sumit Kale** (2019–2023), Chemistry — Quantum computing
- **Rishabh Gupta** (2019–2024), Chemistry — Quantum computing
- **Junxu Li** (2018–2023, Physics — Quantum machine learning
- **Juexiao Wang** (2022–2024), Computer Science — Quantum machine learning
- **Keerthi Kumaran** (2023–2024), Physics — Quantum computing algorithms
- **Yuchen Wang** (2017–2023), Physics — Quantum entanglement
- **Vineet Mohanty** (2017–2020), Mechanical Engineering — Quantum phases
- **Shree Hari Sureshbabu** (2020–2023), ECE — Quantum machine learning
- **Raja Selvarajan** (2017–2023), Physics — Quantum algorithms
- **Rongxin Xia** (2016–2020), Physics — Quantum computing
- **Teng Bian** (2016–2020), Physics — Quantum information
- **Zhanfu Yang** (2018–2019), M.Sc., Computer Science — Quantum machine learning
- **Shuxian Jiang** (2012–2017), Computer Science — Quantum annealing
- **Yudong Cao** (2012–2016), Computer Science — Quantum algorithms
- **Rishabh Chandra** (2012–2014), Mechanical Engineering — Quantum algorithms
- **Cyrus Vandrevala** (2011–2014), Physics — Entanglement in materials

- **Yiteng Zhang** (2011–2016), Physics — Entanglement in biological systems
- **Shu-Hao Yeh** (2010–2015), Chemistry — Quantum coherence in photosynthesis
- **Edwin Antillon** (2009–2012), Physics — Finite size scaling, conformal invariance
- **Anmer Deskin** (2009–2013), Computer Science — Quantum compiler
- **Ross Hellen** (2009–2014), Chemistry — Dimensional scaling
- **Jing Zhu** (2006–2012), Chemistry — Quantum algorithms for global optimization
- **Qi Wei** (2004–2010), Chemistry — Stability of matter, dimensional scaling
- **Hefeng Wang** (2004–2008), Chemistry — Quantum algorithms
- **Winton Moy** (2004–2010), Chemistry — Finite elements and scaling
- **Xu Qing** (2005–2010), Physics — Spin systems
- **Zheng Huang** (2002–2007), Chemistry — Entanglement theory
- **Aaron Stanton** (1995–1999), Chemistry — Global optimization
- **Pablo Nigra** (1996–2001), Chemistry — Water clusters and phase changes
- **Stephen Belair** (1998–2004), Chemistry — Electronic structure methods
- **Imad Ladadwa** (1999), Visiting student — Finite size scaling in scattering theory

Current Postdoctoral Associates

- **Manas Sajjan** (2020–Present) — Quantum transport and quantum computing
- **Amandeep Bhatia** (2021–Present) — Federated quantum machine learning
- **Mandeep Saggi** (2022–Present) — Quantum machine learning
- **Sangbo Xie** (2024–Present) — Quantum algorithms

Former Postdoctoral Associates

- Richard Bleil (1994–1995) Chemistry — Dakota State University
- Pablo Serra (1995–1997) Physics — University of Córdoba
- Juan Pablo Neirotti (1997–1998) Physics — São Paulo
- Alexei V. Seregeev (1998–1999) Physics — Ben Gurion University
- Ricardo Sauerwein (1999–2001) Physics — Federal University of Santa Maria
- Qicun Shi (1998–2005) Chemistry — Research Scientist, MIT
- Jiaxiang Wang (2001–2004) physics — East China Normal University
- Omar Osenda (2002–2004) Physics — University of Córdoba
- Felipe Herrera (2012–Present) Chemistry — Universidad de Santiago de Chile
- Dong Wang (2014–2015) Chemistry — Anhui University
- Sachin D. Yeole (2014–2015) Chemistry — Finite size scaling
- Jiang Wang (2015–2016) Computer Science — Quantum computing
- Nan Jiang (2015–2016) Computer Science — Quantum entanglement
- Merid Legesse Belayneh (2015–2017) Chemistry — Quantum materials
- Shuhao Yeh (2016–2019) Chemistry — Quantum devices
- Kumar Ghosh (2018–2020) Chemistry — Quantum machine learning
- Vivek Dixit (2019–2021) Chemistry — Quantum machine learning

- Yijue Ding (2018–2020) Physics — Quantum entanglement
- Sangchul Oh (2020–2023) Chemistry — Quantum computing algorithms
- Zixuan Hu (2016–2023) Chemistry — Quantum coherence & computing
- Rishabh Gupta (2024–2025), Chemistry — Quantum computing
- Yuchen Wang (2023–2024), Physics — Quantum entanglement

Funded Proposals and Grants

- **A New Approach to Global Minimization**, ACS-PRF **\$20,000** 06/01/1996–08/31/1998 **PI: Sabre Kais**
- **Renormalization Group Approach for the Treatment of Electron Correlation**, PRF **\$5,000**, 07/01/1996–06/30/1997 **PI: Sabre Kais**
- **Critical Phenomena and Renormalization Group Approach for Electronic Structure Calculations**, ONR **\$300,000**, 12/01/1996–09/30/1999 **PI: Sabre Kais**
- **Scaling Theory for Electronic Structure**, NSF CAREER **\$340,000**, 10/15/1998–04/15/2002 **PI: Sabre Kais**
- **Critical Phenomena and Renormalization Group Approach for Electronic Structure Calculations**, ONR **\$300,000** 12/01/1999–09/30/2002 **PI: Sabre Kais**
- **Finite Size Scaling and Stability of Atomic and Molecular Ions**, ACS-PRF **\$80,000** 04/01/2002–08/31/2004 **PI: Sabre Kais**
- **Critical Phenomena and Renormalization Group Approach for Electronic Structure Calculations**, ONR **\$100,000** 09/30/2002–12/01/2004 **PI: Sabre Kais**
- **Scaling Theory for Electronic Structure**, NSF **\$291,000** 02/01/2002–01/31/2006 **PI: Sabre Kais**
- **Dynamics of Entanglement and Decoherence for Quantum Computing**, PRF **\$13,776** 07/01/2005–06/30/2006 **PI: Sabre Kais**
- **Entanglement Production by Electron Transfer Processes in Mesoscopic and Molecular Systems**, BSF/“BNSF” **\$120,000** 07/01/2005–06/30/2010 **PI: Sabre Kais; Co-PI: Uri Peskin**
- **Stability of Multiply Charged Ions by Superintense Laser Fields**, PRF **\$15,292** 06/01/2006–05/31/2007 **PI: Sabre Kais**
- **CPATH CB: Computing Education in Science Context**, NSF **\$446,000** 07/01/2007–06/30/2010 **Co-PI: Sabre Kais**
- **Quantum Phase Transitions for Atoms, Molecules and Quantum Degenerate Gases**, ARO **\$100,000** — 07/01/2007–06/30/2008 **PI: Sabre Kais**
- **Simulated Quantum Computation of Global Optimization**, PRF **\$16,300** 06/01/2008–05/31/2009 **PI: Sabre Kais**
- **Finite Size Scaling and Quantum Criticality of Quantum Gases**, ARO **\$300,000** 01/01/2009–12/30/2012 **PI: Sabre Kais**

- **Quantum Computer Algorithm for Chemistry**, PRF **\$16,300** 06/01/2009–05/31/2010 PI: **Sabre Kais**
- **NSF Centers for Chemical Innovation (Phase I): Quantum Information and Computation for Chemistry** NSF — **\$1,500,000** 10/01/2010–09/30/2013 PI: **Sabre Kais (Purdue)**; Co-PIs: A. Aspuru-Guzik, K. Brown, D. Lidar, P. Love
- **Radical Chemistry on Cloud and Aerosol Surfaces**, NSF **\$775,000** 09/01/2013–08/31/2015 PI: **Joseph Francisco**; Co-PI: **Sabre Kais**
- **New Chemistries for Catalytic Conversion of Natural Gas to Valuable Organics**, Qatar Foundation **\$1,000,000**, 10/01/2013–09/30/2015 PI: **Mahdi Abu Omar**; Co-PI: **Sabre Kais**
- **Quantum Aspects of Non-Adiabatic Electronic Energy Transfer in Photosynthetic Light-Harvesting Complexes**, Purdue–Universidad de Antioquia Seed Grant **\$56,000** 2015–2017 Co-PIs: **Sabre Kais (\$6,000)** and **Leonardo A. Pachón (\$50,000)**
- **Studies of Electron Correlations in Potential-Matched Direct Nonequilibrium Solar Refrigeration**, Qatar Foundation **\$900,000** 10/01/2014–09/30/2017 PI: **Sabre Kais**; Co-PIs: Fahhad Alharbi, Tim Fisher
- **Coherent Energy Transfer in Novel Excitonic Materials for Solar Energy Applications**, Qatar Foundation **\$5,000,000** 01/31/2016–01/30/2021 PI: **Sabre Kais**; Co-PIs: Fahhad Alharbi, Greg Engel
- **Quantum Machine Learning for Data Analytics and Optimization**, Discovery Park (Purdue) **\$300,000** 08/01/2018–08/01/2020 PI: **Sabre Kais**; Co-PIs: Yong Chen, Alex Pothen, Ashraf Alam
- **NSF RAISE-TAQS: High Dimensional Frequency-Bin Entanglement Photonic Integration and Algorithms**, NSF **\$1,000,000** 08/15/2018–08/14/2021 (NCE to 2022) Co-PI: **Sabre Kais**; PI: Andrew Weiner; Co-PI: Minghao Qi
- **Quantum Machine Learning for Extended Systems** U.S. Air Force **\$75,000** 09/01/2020–08/31/2021 (NCE to 2022) PI: **Sabre Kais**
- **Developing Quantum Machine Learning Methods for Computational Chemistry**, ORNL **\$50,000** 09/01/2020–08/31/2021 PI: **Sabre Kais**
- **Quantum Machine Learning for Classifying Entanglement in Complex Systems** PRF / Graduate School Support **\$20,782 (est.)** 2020–2021 PI: **Sabre Kais**
- **Cryptography by Image Reconstruction Using a Quantum Annealer (Seed Project)** Purdue QSEI **\$10,000** Summer 2020 PI: **Sabre Kais**
- **NSF IUCRC Planning Grant: Center for Quantum Technologies (CQT)** NSF **\$20,000** 06/01/2021–12/30/2021 PI: **Sabre Kais (Center Director)**; multi-institution collaboration (Purdue, IU, ND, IUPUI)

- **Quantum Computing Algorithms and Applications for Coherent and Strongly Correlated Chemical Systems** DOE **\$2,475,000** 09/15/2018–09/14/2021 **PI: Sabre Kais**; Co-PIs: D. Mazziotti, Y. Chen, L. Huang, J. Anderson
Renewal: \$3,000,000 09/15/2021–09/14/2024 **PI: Sabre Kais**; Co-PIs: D. Mazziotti, P. Narang, Y. Chen, L. Huang, J. Anderson
- **Resisting Adversarial Attacks with Quantum Machine Learning** Soar Technology, Inc. **\$150,000** 01/04/2020–12/30/2023 **PI: Sabre Kais**
- **Near-Term Applications of Quantum Machine Learning Techniques to Quantum Chemistry**, NSF **\$450,000** 09/01/2020–08/31/2023 **PI: Sabre Kais**
- **Quantum Science Center (DOE Center)** ORNL/QSC **\$115M (Center total)** 2020–2025
Project: Developing quantum algorithms and quantum machine learning for materials **\$750,000** 01/09/2020–08/31/2025 **PI: Sabre Kais**
- **CCI Phase I: NSF Center for Quantum Dynamics on Modular Quantum Devices (CQD-MQD)** NSF **\$1,800,000 (Center total)** 09/01/2021–08/31/2024
Purdue Subaward: \$330,000 Co-PI: **Sabre Kais** (PI: Victor Batista; other Co-PIs: Eitan Geva, Lea F. Santos)
- **IUCRC Phase I: Center for Quantum Technologies (CQT)** NSF IUCRC **\$1,125,000** 09/01/2022–08/31/2027 **PI: Sabre Kais**; Co-PI: David J. Stewart
- **Ford–Purdue Alliance Proposal 001826-PUR: Simulating Battery Materials Using a Hybrid Quantum Algorithm Based on Periodic Restricted Boltzmann Machine** Ford/Purdue **\$2,010,000** 05/01/2023–04/30/2025 **PI: Sabre Kais**
- **Ross–Lynn Research Scholar Grant: Maneuvering Atomic Legos on a Potential Energy Surface Using Quantum-Assisted Neural Network Encoding** Purdue (Graduate student support) 06/2023–12/2023
- **Bilsland Dissertation Fellowship** Purdue Graduate School **2023–2024** (dates as provided; adjust if needed)
- **Quantum Science Seed Grant: Exploiting Topological Phases of Matter** Purdue **\$50,000** 2023–2024 (Team: R. Kaufmann, B. Kaufmann, S. Cui, S. Kais)
- **Quantum Science Center Renewal (SPARK program)** Purdue **\$100,000** (Team: Y. Chen, S. Kais, V. Shalaev, A. Boltasseva)

Current Active Awards at NC State

- **DOE, Developing Non-Equilibrium Dynamical Effects and Emergent Phenomena: Through the Lens of Quantum Information Science, \$750,000** 05/01/2025 - 04/30/2028 **PI: Sabre Kais**
- **QuPIDC Department of Energy (DOE) Energy Frontier Research Center (EFRC)** led by Purdue University and directed by Professor Libai Huang, my grant is

developing quantum computing algorithms for super-radiant phases and photon matter interactions, **\$600,000** 01/09/2024–08/31/2029

- **Quantum Science Center (DOE Center)** ORNL/QSC **\$120M (Center total)** 2024–2030

Project: *Developing quantum algorithms and quantum machine learning for complex systems* **\$1,000,000** 01/09/2025–08/31/2030 **PI: Sabre Kais**

Research Program

My research integrates **quantum computing, quantum chemistry, and quantum machine learning** to develop new algorithms and theoretical frameworks for simulating complex molecular, materials, and many-body quantum systems. The program spans quantum algorithms, hybrid quantum–classical learning, quantum coherence in energy transport, and scaling theory for quantum critical phenomena.

1. Quantum Computing Algorithms for Chemistry and Materials

Developing efficient quantum algorithms for solving electronic structure and many-body problems on gate-based quantum computers.

Contributions include:

- Ground-state algorithms for electronic structure problems
- Circuit-depth and gate-count optimization for Hamiltonian simulation
- Quantum linear-system solvers (e.g., Poisson equation)
- Orders-of-magnitude reductions in circuit complexity via efficient wavefunction emulation
- Practical implementations on NISQ and hybrid architectures

Representative publications:

J. Phys. Chem. B (2018); Quantum Inf. Comput. (2017); Quantum Inf. Process. (2014–2017); J. Chem. Phys. (2012, 2014, 2022); Phys. Rev. A (2014); Sci. Rep. (2018); Commun. Phys. (2022); Phys. Rev. Research (2023); J. Phys. Chem. Lett. (2023); Physical Review B 111 (8), 085303 (2025)

2. Quantum Machine Learning for Molecules and Materials

Pioneering hybrid quantum–classical learning methods for electronic structure, molecular design, and materials discovery.

Key advances:

- Quantum-enhanced restricted Boltzmann machines (RBMs)
- Hybrid quantum neural-network approaches for potential energy surfaces
- Quantum-assisted optimization of molecular ground states
- Band-structure prediction for low-dimensional materials
- Algorithms combining variational circuits with classical ML for scalable accuracy

Representative publications:

Nature Communications (2018); Chemical Society Reviews (2022), Natural Sciences 3 (4), e20230015 (2025)

3. Quantum Coherence and Quantum Transport

Developing theoretical frameworks to understand and exploit coherence effects in energy transport and light-harvesting systems.

Highlights:

- New formalism describing coherence-enhanced transport
- Demonstrated how dark states and cooperative dipole interactions improve photocell efficiency
- Models explaining near-unity photon-to-charge conversion in biological systems
- Design principles for photosynthesis-inspired photovoltaic devices

Representative publications:

PNAS (2018); Chem (2018); J. Chem. Phys. (2018); PCCP (2015–2016); Sci. Rep. (2016); Phys. Rev. E (2013); Quantum (2022); J. Phys. Chem. Lett. (2023); Chemical Reviews 126 (1), 1-3 (2026)

4. Dimensional and Finite-Size Scaling in Quantum Systems

Foundational theoretical work connecting electronic structure theory with quantum critical phenomena.

Contributions:

- Analogy between symmetry breaking in electronic structure and quantum phase transitions
- Finite-size scaling theory for quantum Hamiltonians
- Basis-set scaling as an effective “system size”
- Applications to atomic, molecular, and condensed-matter systems

Representative publications:

Advances in Chemical Physics (2003); J. Chem. Phys. (2022); Frontiers in Physics (2022); Physical Review A 112 (1), 012201(2025)

Teaching

Over 30 years of undergraduate and graduate instruction across chemistry, physics, mathematics, and electrical and computer engineering.

Courses taught include:

- Physical Chemistry
- Modern Physics
- Statistical Mechanics / Statistical Physics
- Quantum Mechanics (introductory and advanced)
- Quantum Chemistry

- Density Functional Theory
- Computational Methods
- Global Optimization
- Quantum Information and Quantum Computing
- Applied Quantum Mechanics for Engineers
- Special Topics in Materials Science and Quantum Technologies

Publications List

1. M.Cohen and S. Kais, Scaling, Renormalization and Accuracy of Perturbation Calculation, *Chem, Phys. Lett.* 105, 295-298 (1984).
2. M. Cohen and S. Kais, Rayleigh-Schrodinger Perturbation Theory with a Strong Perturbation, *J. Phys.* B17, 3049-3055 (1984).
3. M. Cohen, T. Feldman and S. Kais, Stark Effect of a Rigid Rotor, *J. Phys.* B17, 3535-3544 (1984).
4. S. Kais, Unstable Bound States by an Algebraic Method, *Phys. Lett.* 112A, 269-270 (1985).
5. S. Kais and S.K. Kim, Unstable Bound States of the Dirac Equation, *Phys. Lett.* 114A, 165-167 (1986).
6. M. Cohen and S. Kais, Rayleigh-Schrodinger Perturbation Theory with a Strong Perturbation: Anharmonic Oscillator, *J. Phys.* A19 683-690 (1986).
7. R. Gilmore, S. Kais and R.D. Levine, Quantum Cusp, *Phys. Rev* A34, 2442-2452 (1986).
8. S. Kais and R.D. Levine, Square-Well Potential by an Algebraic Approach, *Phys. Rev.* A34, 4615-4621 (1986).
9. S. Kais and R.D. Levine, Directed States of Molecules, *J. Phys. Chem.* 91, 5462-5465 (1987).
10. S. Kais, M. Cohen and R.D. Levine, The Perturbed Hydrogen Atom: Some New Algebraic Results, *J. Phys.* A22, 803-810 (1989).
11. S. Kais, D.R. Herschbach and R.D. Levine, Dimensional Scaling as a Symmetry Operation, *J. Chem. Phys.* 91, 7791-7796 (1989).
12. S. Kais and R.D. Levine, Coherent States for the Mores Potential, *Phys. Rev.* A41, 2301-2305 (1990).
13. J.G. Loeser, Z. Zhen, S. Kais and D.R. Herschbach, Dimensional Interpolation of Hard Sphere Virial Coefficients, *J. Chem. Phys.* 95, 4525-4544 (1991).
14. S. Kais, J.D. Morgan III and D.R. Herschbach, Electronic Tunneling and Exchange Energy in the D-dimensional Hydrogen Molecule Ion, *J. Chem. Phys.* 95, 9028-9041 (1991).
15. S. Kais, D.D. Frantz and D.R. Herschbach, Electronic Tunneling in the Hydrogen-Molecule Ion Evaluated from the Large-dimensional Limit, *Chem. Phys.* 161, 393 402(1992).

16. S. Kais, Symmetry Breaking and Electronic Exchange Energy. In Dimensional Scaling in Chemical Physics, Edited by D.R. Herschbach, J. Avery and O. Goscinski (Kluwer Academic, Dordrecht, Holland, 1992), page 256-273
17. S. Kais and D.R. Herschbach, Dimensional Scaling for Quasistationary States, *J. Chem. Phys.* 98, 3990(1992).
18. S. Kais and G. Beltrame, Dimensional Scaling for Regge Trajectory, *J. Phys. Chem.* 97, 2453-2456 (1992).
19. S. Kais, C.W. Murray, N.C. Handy and D.R. Herschbach, Density Functional and Dimensional Renormalization for an Exactly Solvable Model, *J. Chem. Phys.* 99, 417-425 (1993).
20. S. Kais, S.M. Sung and D.R. Herschbach, Atomic Energies from Renormalization of the Large-Dimension Limit. *J. Chem. Phys.* 99, 5184-5196 (1993).
21. T.C. German and S. Kais, Large Order Dimensional Perturbation Theory for Complex Energy Eigenvalues. *J. Chem. Phys.* 99, 7739-7747 (1993).
22. D.J. Lacks and S. Kais, Statistical Model for Delocalized Pi Bonding in the C₆₀ Molecule, *Chem. Phys. Lett.* 218, 229-233 (1994).
23. S. Kais, S.M. Sung and D.R. Herschbach, Large-Z and -N Dependence of Atomic Energies from Renormalization of the Large-Dimension Limit, *Int. J. Quantum Chem.* 49, 657-674 (1994).
24. S. Kais and D.R. Herschbach, The 1/Z Expansion and Renormalization of the Large-Dimension Limit for Many-Electron Atoms, *J. Chem. Phys.* 100, 4367-4376 (1994).
25. S. Kais, T.C. German, and D.R. Herschbach, Large-Dimension Limit Yields Generic Potential Curves for H₂+, H₂, HHe+, and He₂++, *J. Phys. Chem.* 98, 11015-11017 (1994).
26. R. Bleil, F.M. Tao and S. Kais, Structure and Stability of C₁₃ Carbon Clusters, *Chem. Phys. Lett.* 229, 491(1994).
27. S. Kais and R. Bleil, Charge Renormalization at the Large-D Limit for N-Electron Atoms and Weakly Bound Systems. *J. Chem. Phys.* 102, 7472-7478 (1995).
28. R. Bleil and S. Kais, Charge Renormalization at the Large-D Limit for Atoms and Molecules, *Int. J. Quantum. Chem.* 29, 349-359 (1995).
29. R. Bleil, A. Faliks, M. Miletic and S. Kais, Charge Renormalization at the Large-D Limit for Diatomic Molecules, *J. Chem. Phys.* 103, 6529-6535 (1995).
30. S. Kais and R. Bleil, Dimensional Renormalization for Electronic Structure Calculation in "New Methods in Quantum Theory" NATO Advance Research Workshop, Ed: C.A. Tsipis, V.S. Popov, D.R. Herschbach, and J. Avery. (Kluwer Academic, Dordrecht, Holland, 1996), page 55-70.
31. S.A. Lee, S.Z. Kan, Y.H. Kim, M. Miletic, R. Bleil, S. Kais and B.S. Freiser, Experimental and Theoretical Studies of Nb₆C₇₀+, *J. Phys. Chem.* 100, 6336-6341 (1996).
32. P. Serra and S. Kais, Critical Phenomena for Electronic Structure at the Large-Dimension Limit, *Phys. Rev. Lett.* 77, 466-469 (1996).
33. P. Serra and S. Kais, Multicritical Phenomena for the Hydrogen Molecule at the Large-Dimension Limit, *Chem. Phys. Lett.* 260, 302-308 (1996).

34. P. Serra and S. Kais, Phase Transitions for N-Electron Atoms at the Large-Dimension Limit, *Phys. Rev A.* 55, 238-247 (1997).
35. T.C. Germann and S. Kais, Dimensional Perturbation Theory for Regge Poles, *J. Chem. Phys.* 106, 599-604 (1997).
36. A. Stanton, R. Bleil and S. Kais, A New Approach to Global Minimization, *J. Comp. Chem.* 18, 594-599 (1997).
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306. M. Rose, S. Kais, and D. A. Mazziotti, "Open-Quantum-System Simulation Through Exploiting Noise on Quantum Computers," *Phys. Rev. A* 111, 052612 (2025). DOI: 10.1103/PhysRevA.111.052612
307. L. H. Delgado-Granados *et al.*, S. Kais, and D. A. Mazziotti, "Quantum Algorithms and Applications for Open Quantum Systems," *Chemical Reviews* (2025). DOI: 10.1021/acs.chemrev.4c00428
308. A. Bhatia, S. Kais, and M. Alam, "Quantum Federated Learning in Healthcare: The Shift from Development to Deployment and from Models to Data," *IEEE J. Biomedical and Health Informatics* (2025). DOI: 10.1109/JBHI.2025.3596156
309. M. Mousa, B. Wehefritz-Kaufmann, S. Kais, S. Cui, and R. Kaufmann, "Refined Phase Diagram for a Spin-1 System Exhibiting a Haldane Phase," *Phys. Rev. B* 111, 085303 (2025). DOI: 10.1103/PhysRevB.111.085303
310. T. Aziz, M. Song, L. Ye, D. Wang, J. Gil, and S. Kais, "Spectral Bounds on Entropy and Ergotropy via Statistical Effective Temperature in Classical Polarization and Quantum Thermal States," *Phys. Rev. Research* 7, 033XXX (2025).
311. Z. Hu and S. Kais, "The Qubit Information Logic Theory for Understanding Multi-Qubit Entanglement and Designing Exotic Entangled States," *Annalen der Physik* (2025). DOI: 10.1002/andp.202500176
312. P. Narang, S. Kais, A. Aspuru-Guzik and V. Batista, "Introduction: Quantum Computing", *Chemical Reviews* (2026). 10.1021/acs.chemrev.5c00989
313. Bhatia, A. S., Saggi, M. K., & Kais, S, "Application of quantum-inspired tensor networks to optimize federated learning systems", *Quantum Machine Intelligence*, Vol. 7. (2025), 10.1007/s42484-025-00243-x

Invited Review Articles

- S. Kais, Symmetry Breaking and Electronic Exchange Energy. In Dimensional Scaling in Chemical Physics, Edited by D.R. Herschbach, J. Avery and O. Goscinski (Kluwer Academic, Dordrecht, Holland, 1992), page 256-273.

- S. Kais and R. Bleil, Dimensional Renormalization for Electronic Structure Calculations, in "New Methods in Quantum Theory" NATO Advance Research Workshop, Ed: C.A.Tsipis, V.S. Popov, D.R. Herschbach, and J. Avery. (Kluwer Academic, Dordrecht, Holland, 1996), page 55-70.
- S. Kais, "Exact Models", in "The Encyclopedia of Computational Chemistry," Schleyer, P. v. R.;Allinger, N. L., Clark, T.; Gasteiger, J.; Kollman, P. A.;Schaefer III, H. F.; Schreiner, P. R. (Eds.); John Wiley and Sons: Chichester, 1998, pp. 959-963.
- Sabre Kais and Pablo Serra, "Quantum Critical Phenomena and Stability of Atomic and Molecular Ions", *Int. Rev. Phys. Chem.* Vol 19, 97-121 (2000).
- S. Kais and P. Serra, "Finite Size Scaling for Atomic and Molecular Systems", *Advances in Chemical Physics*, Volume 125, 1-100 (2003).
- Sabre Kais, "Entanglement, Electron Correlation and Density Matrices" Reduced-Density-matrix Mechanics with Applications to Many-electron Atoms and Molecules, *Advances in Chemical Physics* Vol 134, edited by D. A. Mazziotti (Wiley, New York, 2007).
- Sabre Kais and Hefeng Wang, "Quantum Teleportation in Quantum Dots System", *Handbook of Nanophysics*, Edited by Klaus Sattler, (Taylor and Francis, 2012).
- Sabre Kais, "Finite Size Scaling for Criticality of the Schrodinger Equation", "Solving the Schrodinger equation: has everything been tried", Edited by Paul Popelier (Imperial College Press, London, 2013).
- Mikhail Lemeshko, Roman V. Krems, John M. Doyle, Sabre Kais, Manipulation of Molecules with Electromagnetic Fields, *Mol. Phys.* 111, 1648 (2013).
- Fahhad Alharbi and Sabre Kais, Theoretical Limits of Photovoltaics Efficiency and Possible Improvements by Intuitive Approaches Learned from Photosynthesis and Quantum Coherence, *Renewable and Sustainable Energy Reviews* 43, 1073 (2015).
- Yiteng Zhang, Gennady Berman and Sabre Kais, The Radical Pair Mechanism and the Avian Chemical Compass, *Int. J. of Quantum Chemistry*, 115, 15 (2015)
- Hoehn, R.H.; Nichols, D.E.; Neven, H.; Kais, S Status of the Vibrational Theory of Olfaction *Frontiers in Physics*, 6,25 (2018).
- Yuchen Wang, Zixuan Hu, Barry C. Sanders, Sabre Kais, "Qudits and high-dimensional quantum computing", *Frontiers in Physics*, 8, 589504, DOI:10.3389/fphy.2020.589504 (2020)
- Sabre Kais et. al, "Quantum Machine Learning for Chemistry and Physics", Invited by *Chemical Society Reviews* 2022, 51, 6475 DOI:10.1039/D2CS00203E (2022).
- Delgado-Granados, L. H., Krogmeier, T. J., Sager-Smith, L. A. M., Avdic, I., Hu, Z., Sajjan, M., ... Mazziotti, D. A., " Quantum Algorithms and Applications for Open Quantum Systems", *Chemical Reviews*, Vol. 2. (2025).

Books and Special Issues

- Sabre Kais, Quantum Information for Quantum Chemistry, *Adv. Chem. Phys.* Volume 154, (2014).
- Mikhail Lemeshko, Roman V. Krems, John M. Doyle and Sabre Kais, A Festschrift for Bretislav Friedrich, *Mol. Phys.* Volume 111 (2013).

- Bretislav Friedrich, Sabre Kais, David Mazziotti, A., Festschrift for Dudley R. Herschbach, Mol. Phys., Volume 110. (2012).
- Sabre Kais and Nicholas Handy, A. Festschrift for Raphael D. Levine, Mol. Phys., Volume 106 (2008).
- U. Peskin, O. Alon, M. Segev, M and S. Kais, "Quantum Dynamics and Resonances in Chemistry and Physics" to honor Nimrod Moiseyev on his 70th birthday", Mol.. Phys. Volume 117 (2019).
- Sabre Kais, Frontiers in Physics, "Quantum Information and Quantum Computing for Chemical Systems", <https://lnkd.in/ePhqE3Q> 2021.
- Festschrift for Dor Ben-Amotz , The Journal of Physical Chemistry B 126 (16), 2943-2945
- Yuchen Wang, Zixuan Hu, and Sabre Kais, "Photonic Realization of Qudit Quantum Computing". Published in: Photonic Quantum Technologies: Science and Applications Edited by M. Benyoucef (WILEY-VCH 2023).
- Joseph S. Francisco Festschrift, The Journal of Physical Chemistry (2026).

Invited Lectures

1. "Quantum Batteries", Battery and Energy Storage Symposium, NC State University, Raliegh, Tuesday, Jan. 20, 2026.
2. "Information scrambling and the learning landscape of a quantum machine learning Algorithm", Department of Physics and Astronomy at the University of North Carolina (U NC) January 12, 2026
3. "Information scrambling and the learning landscape of a quantum machine learning Algorithm", International Workshop on Quantum Boltzmann Machines, Dec. 8-11, 2025 Ithaca, NY, USA, Guangzhou, Guangdong, China
4. "Simulation of Chemical Reactions on a Quantum Computer", The 2025 North Carolina Photochemistry Symposium, November 8, 2025, NC State University.
5. "Quantum Machine Learning for AI", October 30, 2025, Applied Materials, Santa Clara California, USA
6. "Quantum - Opportunities / Key Activities and Resources at NC State", Exploring Breakthroughs in Semiconductors and Quantum Computing", A joint workshop by NC State-College of Engineering and Applied Materials, Wednesday, October 8, 2025, Santa Clara CA.
7. "Information scrambling and the learning landscape of a quantum machine learning algorithm", First International Quantum Horizons Symposium at the Banff Centre, August 20-22,(2025) Banff, Canda.
8. "Modulator-Assisted Local Control of Quantum Battery via Zeno Effect", QC-Horizon 2025: Quantum Informatics, Computing & Technology 2025, August 26, 2025.

9. Quantum Machine Learning and Implementation on Quantum Devices for Complex Chemical Systems" town hall, NSF Q-Blue Project, Iowa State University , " June 11-12 (2025).
10. Dirac Quantum Discussions, " Quantum Machine Learning for Complex Chemical Systems", Florida State University, February 25-27, 2025.
11. The 9th US-Japan Digital Innovation Hub and Advances Technology Workshop, "Quantum technologies", at Sophia University, Tokyo Japan, July 19, 22, 2025 .
12. SAS meeting, "NC State Quantum Computing", SAS Campus Cary, NC, July 28th , 2025
13. Qudits for Quantum Technology Workshop, "2024 "Simulation of Chemical Reactions on a Quantum Computer" University of Waterloo, IQC , July 9-11, 2024.
14. American Conference on Theoretical Chemistry 2024 "Simulation of Chemical Reactions on a Quantum Computer" June 17-20, 2024 Chapel Hill, North Carolina.
15. King Fahd University of Petroleum and Minerals (KFUPM) , , "Information scrambling and the learning landscape of a quantum machine learning algorithm", June 5, 2024 Dhahran, Saudi Arabia
16. 4th Annual Quantum Summer School, " "Simulation of Chemical Reactions on a Quantum Computer" APRIL 30TH – MAY 3RD, 2024 Hosted by Purdue University
17. Berkeley, Collage of Chemistry, Physical Chemistry Seminar, "Journey with Quantum Information and Computing for Complex Chemical Systems", March 19, 2024.
18. Rochester Center for Coherence and Quantum Optics Colloquium, "Information scrambling and the learning landscape of a quantum machine learning algorithm", November 30th 2023, Univ. Rochester .
19. Duke Quantum Center, "Information scrambling and the learning landscape of a quantum machine learning algorithm", October 12, Durham, NC.
20. IEEE Quantum Week, WKS10 — Chemical Applications of Quantum Computing, " "Quantum Machine Learning for Complex Chemical Systems", Sept. 18, Seattle, WA.
21. IEEE Quantum Week, WKS12 — Quantum Artificial Intelligence,),"Information scrambling and the learning landscape of a quantum machine learning algorithm", Sept. 19, Seattle, WA.
22. Oak Ridge national Laboratory (ONRL), "Information scrambling and the learning landscape of a quantum machine learning algorithm", August 25, 2023.
23. Caltech, AWS -Chan quantum group "Information scrambling and the learning landscape of a quantum machine learning algorithm" Wednesday July 27, Pasadena, CA.

24. UC San Diego, “Quantum Machine Learning for Complex Chemical Systems”, July 28, San Diego, CA.
25. UC Santa Barbara, “Quantum Machine Learning for Complex Many-Body Systems on Quantum Devices”, July 19, Santa Barbara, CA.
26. UCLA, “Quantum Machine Learning for Complex Many-Body Systems on Quantum Devices”, July 12, Los Angeles, CA.
27. UC Irvine, “Quantum Machine Learning for Complex Many-Body Systems on Quantum Devices”, July 6, Irvine, CA.
28. Virtual Learning University, “Quantum Machine Learning for Complex Many-Body Systems on Quantum Devices”, June 3.
29. Air Force Research Laboratory (AFRL) and Air Force Institute of Technology, “Quantum machine learning for complex chemical systems”, May 12, 2023. Dayton, OH.
30. 3rd Annual Quantum Summer School, “Information Scrambling and the Learning landscape of a Quantum Machine Learning Algorithm”, April 27-30th 2023, Purdue.
31. ACS 2023, “Quantum Information and Quantum Computing for Chemistry” The Second Quantum Revolution: Introduction to Quantum Information and Quantum Computing March 25th 2023, Indianapolis.
32. ACS 2023, “Quantum Information and Quantum Computing for Chemistry”, “Introduction to Quantum Information and Quantum Computing for Chemistry”, March 25th 2023, Indianapolis.
33. Quantum machine learning for complex chemical systems, Department of Chemistry, Northwestern, Center for Molecular Quantum Transduction (CMQT) , March 2nd , 2023
34. Quantum many-Body Simulations of Interesting States of Matter Workshop, “*Information scrambling for navigating the learning landscape of a quantum machine learning model*”, CIQC and Quantum Science Center, December 7, 2022, UC Berkeley
35. *IBM Quantum Computing Workshop*, December 9, 2022 IBM Research Almaden in San Jose, California.
36. Physical Chemistry Seminar, “*Quantum Machine Learning for Complex Chemical Systems* “ November 30, 2022, Purdue
37. Quantum Techniques in Machine Learning 2022, “*Information scrambling for navigating the learning landscape of a quantum machine learning model*”, Naples, Italy 7-12 November 2022.
38. Quantum Machine Learning for Quantum Materials, 12t International Advances in Applied Physics, Keynote Speaker, Oludeniz, Turkey , October 13, 2022.

39. Quantum Machine Learning for Complex Many-Body Systems, Illinois Quantum Information Science and Technology Center, University of Illinois, Urbana Champaign, October 4, 2022.

40. Quantum AI Workshop at IEEE Quantum Week 2022, “Imaginary Components of Out-of-Time Correlators and Information Scrambling for Navigating the Learning Landscape of a Quantum Machine Learning Model”, Denver Sept. 21 2022.

41. New Trends in Computational Chemistry – ed. 2022, “Quantum Machine Learning for Complex Many-Body Systems” Spain, Sept 8, 2022..

42. CCI Conference at Yale, “Quantum Machine Learning for Complex Chemical Systems” Yale, August 27, 2022.

43. ACS Fall meeting, Chicago, “Quantum Machine-Learning for Quantum Materials”, August 23, 2022.

44. Hebrew University-Israel, “Quantum Machine-Learning for Complex many-Body Systems on Quantum Devices”, August 18, 2022.

45. Technion-Israel, “Quantum Machine-Learning for Complex many-Body Systems on Quantum Devices”, August 16, 2022.

46. CCP2022, 3rd IUPAP Conference on Computational Physics, Quantum Information and Computation for Complex Chemical Systems”, August 4, 2022.

47. 2022 International Symposium on Quantum Computing: Circuits Systems Automation and Applications (QC-CSAA) <https://qccsaa.com/>. “Quantum Machine Learning for Complex Chemical systems on Quantum Devices” July 18, 2022. Knoxville, TN, USA

48. Ford Research Center, “Quantum Machine Learning for Complex Chemical systems on Quantum Devices”, June 29, 2022. Ford Company, USA

49. QSCP 2022 – 25th International Workshop on Quantum Systems in Chemistry, Physics and Biology, “Quantum Machine Learning for Complex Chemical systems on Quantum Devices”, 19-24 June 2022, Toruń, Poland

50. TSRC-Quantum Frontiers in Molecular Science, June 6-June 10, 2022, “Quantum Machine Learning for Complex Chemical systems on Quantum Devices”, June 8, 2022.

51. Center for Quantum Information and Control, Quantum Machine Learning for Materials”, May 18, 2022.

52. ACS Spring Meeting San Diego, “Quantum Machine-Learning algorithm for evaluating electronic structure of molecules and materials”, March 20, 2022.

53. APS March Meeting, Chicago, “Quantum Machine-Learning algorithm for Complex Chemical Systems, Chicago, March 13, 2022.

54. 61st Sanibel Symposium, “Quantum machine Learning for Complex Chemical Systems”, St. Simons Island, GA Feb. 13, 2022

55. Quantum Information in chemistry, CUNY Graduate Center, Initiative for the Theoretical Sciences, “Quantum machine learning for electronic structure calculations”, Dec. 3, 2021.
56. MIT, Physical Chemistry Seminar, Quantum information and quantum computing for complex systems”, November 2, 2021.
57. UIPD (Innovative Approaches to University-Industry Collaboration) Webinar, Purdue Center for Quantum technology”, Nov. 8, 2021.
58. Center for Quantum Technology (CQT) at Purdue, Planning Meeting, CQT Vision, Capabilities, Value Proposition and Workforce Development”, September 30, 2021.
59. Virtual Learning University, Morocco, Quantum information and quantum computing for complex systems”, October 16, 2021.
60. The Solemn plenary session on “Quantum Commuting”, February 22-24, 2022, of The Hassan II Academy of Science and Technology, Morocco.
61. Boeing, “Quantum Machine Learning for Complex Systems”, Wednesday, September 22, 2021
62. IBM Qiskit Series, Quantum Machine Learning for Complex Chemical Systems”, Friday August 27, 2021.
63. ACS Meeting, “Quantum machine learning for electronic structure calculations of 2D materials on quantum computing devices” Synergy Between Quantum Computing and High-Performance Computing in Quantum Chemistry and Materials Science”, April 12, 2021.
64. ONLINE Lorentz-CECAM workshop 'Useful Quantum Computing for Quantum Chemistry' (22-26 February 2021), Quantum Algorithms for Evolving Open Quantum Dynamics, Feb. 25th , 2021.
65. Purdue University, MacCoy Award Distinguished Lecture, Quantum Information and Quantum Computing for Complex Chemical Systems, October 28, 2019.
66. Harvard University, Department of Physics (Harvard Quantum Initiative) , “Quantum Machine Learning for Complex Systems”, November 6, 2019.
67. Colloquium at the Department of Chemistry and Computer Science, “Quantum Information and Quantum Computing for Complex Chemical Systems”, Marquette University, Milwaukee, WI, September 27, 2019.
68. DOE PIs meeting, “Quantum Computing Algorithms and Applications for Complex Chemical Systems”, Gaithersburg Maryland, May 21-24, 2019.
69. Argonne National Lab, Quantum Information and Computation for Chemistry, Chicago, May 7, 2019.
70. Yale University , Quantum Information and Computation for Chemistry, May 3, 2019.
71. International Symposium of Quantum Science and technology at Purdue, “Quantum Computing for Chemistry”, April 21-23, 2019.

72. Purdue-IU Quantum workshop, “Quantum Algorithms for Chemistry, Feb. 26, 2019.
73. The 59th Sanibel Symposium “Quantum Computing for Complex Chemical Systems” Quantum Theory Project, University of Florida, February 17 - 22, 2019.
74. NSF workshop “Quantum algorithms for quantum chemistry and materials “Quantum Information and Computing for Chemistry “The Blessings and Curses of Dimensionality” Jan 22-24, 2019.
75. NSF “Quantum Computing Workshop”, Nov. 7, 2018. Quantum Computing for chemistry.
76. NIST workshop on Complex Systems Chemistry, Gaithersburg, Maryland, “Quantum Information and Computing for Chemistry”, October 22-24, 2018.
77. National Academies of Sciences, Engineering & Medicine, Chemical Sciences Roundtable, “Quantum Computing”, Friday, July 27, 2018.
78. Israeli Academy of sciences, Quantum Machine Learning for Electronic Structure, June 18, 2018, Jerusalem.
79. Air Force Institute of Technology 2950 Hobson Way WPAFB OH, “Near term applications of small scale quantum computing for quantum chemistry”, May 3, 2018.
80. IBM-Zurich, “Near term applications of small scale quantum computing for quantum chemistry”, June 6, 2018.
81. “Cold molecules for chemistry” symposium at ACS Spring meeting, “Quantum computing with polar molecules”, March 18-20 2018.
82. NASA, Lockheed-Martin center for Innovation, Suffolk, VA, Near term applications of small scale quantum computing for quantum chemistry, November 7, 2017.
83. Department of Chemistry, University of Chicago, Near term applications of small scale quantum computer”, October 24, 2017.
84. 254th ACS Meeting, Mapping electronic structure Hamiltonian to an Ising type Hamiltonian , August 20-21, 2017.
85. Department of Physics, Purdue University, “Near term applications of small scale quantum computer”, April 27, 2017.
86. APS, March Meeting 2017, Chairing the Session “Near term applications of small scale quantum Computing”, New Orleans, March13-17, 2017.
87. Department of Computer Science, Purdue University, “Near term applications of small scale quantum computer”, February 27, 2017.
88. Department of Mathematics, Purdue University, “Near term applications of small scale quantum computer”, February 10, 2017.
89. Wabash College, Department of Physics, Crawfordsville, IN 47933, “Near term applications of quantum computing”, February 6, 2017.
90. Oak Ridge National Laboratory, Quantum Information and Computation: Second Quantum Technology Revolution, January 11, 2017.
91. Zurich IBM Research Laboratory, Adiabatic Quantum Computing, January 25, 2017.

92. Competence Center for Computational Chemistry of the University of Zurich, ETH Zurich, and the Zurich IBM Research Laboratory, Challenges of Electronic Structure calculations on Quantum Computers, January 26, 2017.

93. Challenges of Electronic Structure Calculations on Quantum Computers, Department of Chemistry, Purdue University, November 16, 2016.

94. Freie Universität Berlin, Challenges of Electronic Structure calculations on Quantum Computers, October 4, 2016.

95. Department of Chemistry, University of Virginia, Quantum Information and Quantum Computation for Chemistry, September 30, 2016.

96. Department of Computer Engineering, Istanbul Medeniyet University, Kadikoy, Istanbul, Turkey, Light Matter Interaction: The role of quantum coherence, April 5, 2016.

97. Swiss Chemical Society, Fall Meeting 2015, Lausanne, Challenges of Electronic Structure Calculations, Sept. 4, 2015.

98. Midwest Theoretical Chemistry Conference at the University of Michigan, Challenges of Electronic Structure Calculations on a Quantum Computer, June 26-28, 2015 in Ann Arbor, Michigan

99. KAUST, Saudi Arabia, "Light matter interactions", April 29, 2015.

100. Qatar Foundation, "New Challenges for Electronic Structure calculations", April 13, 2015.

101. Swiss Chemical Society, Fall Meeting 2014, Zurich, Light Matter Interaction, Sept. 11, 2014.

102. IBM Zurich, Switzerland, Challenges of Electronic Structure Calculations for Atoms and Molecules, Zurich, Switzerland, Feb. 26, 2014.

103. Laboratory of Physical Chemistry, ETH, Quantum Coherence and Light matter Interaction, ETH, Zurich, Switzerland, Feb. 27, 2014.

104. Physics and Engineering ICube Laboratory/CNRS, University of Strasbourg, Light Matter Interaction : The role of quantum coherence, Strasbourg, France, Feb. 24, 2014

105. State Key Laboratory of Precision Spectroscopy East China Normal University, Challenges of Electronic Structure Calculations for Atoms and Molecules", Shanghai, China Dec. 1, 2013.

106. China Academy of Engineering Physics, Light Matter Interaction, Mianyang, China Dec. 3, 2013

107. China Academy of Engineering Physics, The Role of Quantum Coherence in Different Systems , Mianyang, Dec. 4, 2013

108. Sigma Xi Award Lecture, Quantum Information for Quantum Chemistry, Purdue, March 25, 2013.

109. Winter School on Quantum Information Science, Feb 28-March 2, 2013, National Cheng Kung University Talks: (1) Quantum Algorithms for Electronic Structure (2) Calculations Quantum Entanglement for Complex Systems (3) Quantum Computing with Polar Molecules

110. APS March Meeting 2013, March 18 - March 22, Baltimore, Maryland Tutorial 4 Quantum Information and Computation for Quantum Chemistry.

111. Santa Fe Institute, Quantum Coherence and Entanglement in Complex Systems, April 6, 2012
112. Los Alamos National Lab, Quantum Entanglement, April 5, 2012.
113. Quantum Computation for Quantum Chemistry: Status, Challenges, and Prospects, Microsoft Research Redmond, Nov, 12, 2012, Redmond, WA
114. Winter School 2012, Quantum Information and Computation for Quantum Chemistry, January 5-7, 2012 at Indian Wells, CA
115. Banff Meeting, BIRS workshop on Quantum Information for Quantum Chemistry, June 6-11, 2011, Banff, Canada.
116. 241st ACS meeting, Division of Physical Chemistry, Anaheim, CA, Tuning and Quenching Entanglement of Dipole Arrays, March 30, 2011
117. Computer Science Department, Purdue University, Quantum Information and Quantum Computation, March 9, 2011.
118. Department of Physics, King Saud University, Riyadh, Saudi Arabia, Finite Size Scaling and Stability of Atomic and Molecular Systems in Super intense Laser Fields. December, 19, 2010.
119. King Abdullah Institute for Nanotechnology, Riyadh, Saudi Arabia, Research Projects in Birck Nanotechnology Center at Purdue, December 20, 2010
120. Department of Physics (Malaz), King Saud University, Riyadh, Saudi Arabia, Quantum Information and Quantum Computation: Toward Realizing a Quantum Computer, December, 21 2010.
121. Department of Physics, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia, Finite Size Scaling, December 25, 2010.
122. Department of Physics, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia, Quantum Information and Computation, December 26, 2010
123. Department of Physics, East China Normal University, China, Finite Size Scaling and Quantum Criticality, November 25, 2010
124. Chinese Academy of Engineering Physics, Mianyang, China, Stability of Atomic and Molecular Systems in Superintense Laser Fields, November 26, 2010.
125. Purdue University, Computer Science, ``Quantum Information and Quantum Computation", October 6, 2010.
126. TMAU-Princeton Summer Workshop on Quantum Optics and Molecular Physics, Quantum Information for Quantum Chemistry\ Casper, Wyoming, July 25-31, 2010.
127. TMAU-Princeton Summer Workshop on Quantum Optics and Molecular Physics, Finite Size Scaling and Quantum Criticality at the Large-D Limit and D=3" Casper, Wyoming, July 25-31, 201
128. TMAU-Princeton Summer Workshop on Quantum Optics and Molecular Physics, Open Problems and Prospects for Linking D-Scaling with other Methods Casper, Wyoming, July 25-31, 2010.
129. Chair: 42nd Midwest Theoretical Chemistry Conference, Department of Chemistry, Purdue, May 20-22, 2010.
130. Department of Physics, Purdue, Quantum Information for Quantum Chemistry", February 11, 2010.

131. The 41st Midwest Theoretical Chemistry Conference, ``Finite Size Scaling and Quantum Criticality", Southern Illinois University, Carbondale Illinois, May 28-30, 2009.
132. Rutgers University, THE 101ST STATISTICAL MECHANICS CONFERENCE, ``Finite Size Scaling in Quantum Mechanics", SUNDAY - TUESDAY, MAY 10-12, 2009.
133. University of Waterloo, Department of Chemistry and the Institute for Quantum Computing (IQC), "Suppose We Build a Quantum Computer, How Chemistry Can Benefit From Such a Computer", March 18, 2009.
134. Fritz Haber Institute of the Max Planck Society, Department of Molecular Physics, Berlin, Germany" Finite Size Scaling and Quantum Criticality", December 12, 2008.
135. Ruhr University, Institute for Theoretical Chemistry, Bochum, Germany" Finite Size Scaling and Quantum Criticality", December 3, 2008.
136. Atomic Physics Workshop 2008, Max Planck Institute for Physics of Complex Systems, Dresden, Germany" Finite Size Scaling in Atomic and Molecular Physics", November 24-28, 2008.
137. Technical University of Dresden, Department of Physics," Finite Size Scaling and Quantum Computing", November 13, 2008.Techical University of Munich, Institute for Measurement Systems and Sensor Technology, Munich, Germany," Finite Size Scaling and Quantum Computing", October 22, 2008.
138. University of Heidelberg, Institute for Theoretical Chemistry, Universitaet Heidelberg, Germany," Finite Size Scaling and Quantum Criticality", October 20, 2008.
139. Freie Universitaet Berlin, Department of Chemistry, Berlin, Germany" Finite Size Scaling in Quantum Mechanics", September 10, 2008.
140. Max Planck Institute for Physics of Complex Systems, Dresden, Germany" Quantum Criticality", August 22, 2008.
141. University of Chicago, James Franck Institute (JFI), "Suppose We Build a Quantum Computer, How Chemistry Can Benefit From Such a Computer", June 10, 2008.
142. Santa Fe Institute, ``Finite Size Scaling and Quantum Criticality", February 7, 2008.
143. Harvard-MIT-BU-BC Theory Seminar, ``Finite Size Scaling in Quantum Mechanics", November 26, 2007.
144. Purdue University, Electrical and Computer Engineering, Nano501`` Finite Size Scaling and Quantum Criticality", November 12, 2007.
145. Illinois Institute of Technology, Physical Sciences, `` Finite Size Scaling for Atomic and Molecular Systems", October 25, 2007.
146. Illinois Institute of Technology, Chemical Engineering, `` Quantum Phase Transition and Stability of Atomic and Molecular Systems", September 5, 2007
147. Technion-Israel, Department of Chemistry, ``Finite Size Scaling in Quantum Mechanics", June 24, 2007.
148. Lewiner Institute of Theoretical Physics, Technion-Israel, Correlated Electrons Day, ``Finite Size Scaling in Quantum Mechanics", June 21, 2007.
149. Yarmouk University, Jordan, ``Quantum Phase Transition and Stability of Atomic and Molecular Systems", May 29, 2007.
150. APS March Meeting 2007, Denver, Colorado, March 5-9, 2007.Session W21: General Theory: Electronic Structure and Interactions", Finite Size Scaling with Gaussian Basis Set"

151. Princeton-TAMU Foundations of Quantum Mechanics Symposium, ``Dimensional Scaling for Stability of Atomic and Molecular Systems", Princeton, 16-17 February 2007.
152. Department of Chemistry, Purdue University, West Lafayette "Finite Size Scaling for Stability of Atomic and Molecular Systems", February 7, 2007.
153. 38th Midwest Chemistry Conference, 'Entanglement and electron Correlation in Quantum Chemistry calculations", Ohio State University Campus, Columbus Ohio, June 15-17, 2006
154. The 36th Winter Colloquium on the Physics of Quantum Electronics," Entanglement as a measure of electron-electron correlation", Snowbird, Utah, January 2-6, 2006.
155. 230th ACS meeting, Washington DC, Aug. 28-Sept. 1, 2005, "Finite Size Scaling for Critical Phenomena in Negative Ion Clusters"
156. Casper College-Texas A M University Quantum Optics Summer Workshop, August 14- August 20, 2005, "Finite Size Scaling in Quantum Mechanics"
157. University of Berkeley, Berkeley, CA Department of Chemistry and Pitzer Center for Theoretical Chemistry. June 24, 2005. Berkeley Quantum Information and Computation Seminar, "Tuning Entanglement for Magnetic Systems"
158. Stanford University, CA, Department of Chemistry, June, 23, 2005, "Finite Size Scaling in Quantum Mechanics"
159. Purdue University, Computer Science and Engineering Spring 2005 Seminar Series, April 27, 2005 "Quantum Computing"
160. Department of Chemistry, Purdue University, West Lafayette "Finite Size Scaling in Quantum Mechanics", March 9, 2005
161. JSPS-PRISM-TAMU Symposium on Quantum materials Science, in the Honor of Prof. Dudley Herschbach, Princeton, 21-22 February 2005."Critical Phenomena at the Large Dimensional Limit"
162. Department of Chemistry, Technion Haifa 32000, Israel, July 27, 2004 "Tuning the Entanglement for magnetic Systems"
163. Department of Chemistry, Technion Haifa 32000, Israel, July 25, 2004 "Finite Size Scaling and Stability of Atomic and Molecular Ions"
164. Department of Chemistry, Purdue University, West Lafayette "Finite Size Scaling in Quantum Mechanics", March 24, 2004.
165. Kansas State University, Department of Chemistry Manhattan KS 66506-3701,"Finite Size Scaling for Stability of Atomic and Molecular Systems", March 18, 2004
166. WISICT 2004, Winter International Symposium on Information and Communication Technologies, Cancun, Mexico, January 5th-8th, 2004"Scaling of Entanglement at Quantum Phase Transitions"
167. WISICT 2004, Winter International Symposium on Information and Communication Technologies, Cancun, Mexico, January 5th-8th, 2004Chair: Workshop on Quantum Information Processing
168. Department of Mathematics, Purdue University, West Lafayette "Finite Size Scaling in Quantum Mechanics", October 3, 2003.
169. NASA JET PROPULSION LABORATORY, California Institute of Technology,"Scaling of Entanglement at Quantum Phase Transitions", August 15, 2003.

170. Workshop on Quantum Computing, "Tuning the Entanglement for magnetic Systems", University of Notre Dame, Notre Dame, IN, August 7, 2003
171. Ohio Section of the APS Spring Meeting, April 11-12, 2003 Michigan State University, "Tuning the Entanglement for a 1D magnetic System with Anisotropic Coupling and Impurities"
172. International Symposium on Frontiers in Molecular Science 2002,Ocean University of Qingdao, China, July 15-18, 2002 (invited by Dr. Shu-Kun Lin, Chairman of the Executive Committee)
173. Florida State University, Department of Chemistry, "Quantum Critical Phenomena and Stability of Atomic and Molecular Ions"(invited by Prof. Sanford Safron)
174. The University of British Columbia, Department of Chemistry, Vancouver, Canada, June 10, 2002"Finite Size Scaling and Renormalization Group for Quantum Critical Phenomena"
175. The 85th Canadian Society for Chemistry (CSC) Vancouver, June 1 to 5, 2002 , computational chemistry symposium, "Quantum Critical Phenomena and Stability of Atomic and Molecular Ions"
176. 2002 DAMOP Annual Meeting, May 29-June 1 Williamsburg, VA meeting of the "Finite Size Scaling for Atomic and Molecular Systems"
177. University of Wisconsin-Madison, Department of Chemistry, Madison, WI, May 20, 2002, "Quantum Phase Transitions and Stability of Atomic and Molecular Systems"\
178. ONR Program Review, Arlington, Virginia, April 30- May 3, 2002"Critical Phenomena and Renormalization Group Approach for Electronic Structure calculations"
179. Yale University, Department of Physics, New Haven, CT, April 22, 2002 "Finite Size Scaling for Quantum Critical Phenomena"
180. Carnegie Mellon University, Department of Chemistry, Pittsburgh, Pennsylvania, April 11, 2002."Quantum phase transitions and Stability of atomic and molecular systems"
181. APS March Meeting 2002, Indianapolis, IN, March 18, 2002Session A31 (Chemical Physics of Complex Systems)"Finite Size Scaling in Quantum Mechanics"
182. APS March Meeting 2002, Indianapolis, IN, March 20, 2002Session M20 (One Dimensional Theory)"Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
183. Sanibel Symposium 2002 in Quantum Chemistry, Florida, February 23, 2002, Chair of plenary session on Multi-Scale Simulation.
184. Illinois Institute of Technology, Department of Biological, Chemical and Physical Sciences, Chicago, IL, February 20, 2002"Finite Size Scaling for Quantum Critical Phenomena"
185. Purdue University, CS\& E Spring 2002 Seminar Series, February 13, 2002 "Finite Size Scaling for Quantum Critical Phenomena"
186. Department of Chemistry, University of Michigan, Ann Arbor, MI, November 8, 2001"Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
187. Department of Chemistry, Wayne State University, Detroit, MI, November 7, 2001"Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
188. Department of Chemistry, Rutgers University, Piscataway, NJ, June 19, 2001"Quantum Phase Transitions and Stability of Atomic and Molecular Systems"

189. Sanibel Symposium 2001 in Quantum Chemistry Florida, February 28, 2001 "Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
190. Purdue University, Department of Chemistry West Lafayette, IN, January 17, 2000 "Quantum Phase Transitions and Stability of Atomic and Molecular Ions".
191. Department of Chemistry, Hebrew University, Jerusalem Israel, November 28, 2000 "Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
192. Department of Chemistry, Ben Goroun University, Israel November 15, 2000 "Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
193. Advances in Finite Time Thermodynamics, Jerusalem, Israel November 12-14, 2000 "Quantum Phase Transitions at $T=0\$$ ".
194. 2000 Midwest Thermodynamics and Statistical Mechanics Conference, Minneapolis, Minnesota, May 14-16, 2000. "Finite Size Scaling for Critical Parameter of Simple Diatomic Molecules"
195. Department of Chemistry, Wabash College, Crawfordsville, IN 47933, Tuesday Feb. 29, 2000 "Recent Advances in Electronic Structure Theory".
196. Department of Chemistry, Indiana University Bloomington, Indiana 47405, Thursday, September 23, 1999 "Phase Transitions and Stability of Atomic and Molecular Ions."
197. Department of Chemistry and Physics, Indiana University, Bloomington, Indiana 47405, Friday, September 24, 1999 "Finite Size Scaling in Quantum Mechanics".
198. Technion, Department of Chemistry Haifa 32000, Israel, Sunday June 13, 1999 "Recent Advances in Density Functional Theory".
199. The Ohio State University Department of Chemistry Columbus, OH 43210, Monday, April 26, 1999 "Phase Transitions and Stability of Atomic and Molecular Ions".
200. Purdue University, Department of Physics, West Lafayette, IN, January 29, 1999 "Phase Transitions and Stability of Atomic and Molecular Ions".
201. University of Illinois at Urbana-Champaign, Department of Chemistry Urbana, IL, December 2, 1998 "Phase Transitions and the Stability of Atomic and Molecular Ions".
202. Purdue University, Department of Chemistry West Lafayette, IN, September 7, 1998 "Phase Transitions and Stability of Atoms and Molecules".
203. 31st Midwest Theoretical Chemistry Conference Department of Chemistry, Purdue University Chair of the Conference.
204. University of California UCLA, Department of Chemistry Los Angeles, CA, March 11, 1998 "Phase Transitions and Stability of Atoms and Molecules".
205. The American Physical Society - 1998 March Meeting, Los Angeles, CA 16-20 March, 1998 "Phase Transitions and Stability of Atomic and Molecular Negative Ions".
206. Southern Methodist University Department of Chemistry Dallas, Texas, April 23, 1998 "Phase Transitions and Stability of Atoms and Molecules".
207. Hebrew University, Department of Chemistry Jerusalem, Israel, December 22, 1997 "Phase Transitions and Stability of Atoms and Molecules".
208. Technion, Department of Chemistry Haifa, Israel, December 23, 1997 "Phase Transitions and Stability of Atoms and Molecules".

209. Ninth Annual Conference on Recent Developments in Electronic Structure Methods Cornell University, Ithaca, NY, May 31-June 2, 1997 "Finite Size Basis Set Scaling Anstaz for Atoms".
210. 30th Midwest Theoretical Chemistry Conference University of Illinois, Urbana-Champaign, May 22-24, 1997 "Comparison of Pivot Methods for Global Optimization
211. The American Physical Society - 1997 March Meeting Kansas City, MO 17-21 March, 1997 "A New Approach for Global Optimization".
212. 29th Midwest Theoretical Chemistry Conference Indiana University-Purdue University Indianapolis, May 30- June 1, 1996" A New Approach to Global Minimization".
213. The American Physical Society: Atomic, Molecular and Optical Physics Indianapolis, Indiana, April 2, 1996"Critical Phenomena for Electronic Structure at the Large-D limit".
214. The University of Illinois at Chicago Department of Chemistry Chicago, Illinois, March 7, 1996 "Dimensional Renormalization for the Treatment of Electron Correlation".
215. Purdue University: The Dean's Freshman Honors Seminar (SCI 110), Nov. 20, 1995 "New Challenges in Quantum Chemistry".
216. Molecular Quantum Mechanics: Methods and Applications University of Cambridge, England, 3-7 September 1995"Charge Renormalization at the Large-D Limit for Electronic Structure Calculations".
217. Technion, Physics Department Haifa, Israel, June 13, 1995 "Dimensional Renormalization for Electronic Structure of Atoms and Molecules".
218. Regensburg University, Institute for Theoretical Chemistry Regensburg, Germany, May 22, 1995"Dimensional Renormalization for Electronic Structure of Atoms and Molecules".
219. NATO Advanced Research Workshop on New Methods in Quantum Theory Halkidiki, Greece, May 14-19, 1995 "Dimensional Renormalization for Electronic Structure Calculations".
220. Northwestern University, XXVIII Midwest Theoretical Chemistry Conference Evanston, Illinois, May 11-13, 1995 "Charge Renormalization at the Large-D Limit for Electronic Structure Calculations".
221. Purdue University, Department of Physic West Lafayette, IN March 20, 1995 Molecules and Clusters".
222. Oregon State University, Department of Chemistry Corvallis, Oregon, April 14, 1993"Electronic Structure Calculations by Density Functional Theory and Dimensional Scaling Methods".
223. Harvard University, Dudley Herschbach's 60th Birthday Cambridge, MA, July 1992 "Dimensional Scaling the Quasi stationary States".
224. Cambridge University, Department of Chemistry Cambridge, England, June 1992"Electronic Structure Calculations by Density Functional and Dimensional Scaling".

- 225. Cornell University, Department of Physics Ithaca, NY, March 3, 1992 "Electronic Structure Calculations by Density Functional and Dimensional Scaling".
- 226. M.I.T., Department of Chemistry Cambridge, MA, October 30, 1991 "Tunneling in Multi-Dimensional Systems".
- 227. New York University, Department of Physics New York, New York, October 21, 1991 "Dimensional Scaling Method in Atomic and Molecular Physics".
- 228. Orstead Institute, Department of Chemistry Copenhagen, Denmark, June 1991 Conference in Dimensional Scaling in Chemical Physics "Symmetry Breaking and Electronic Exchange Energy".

Other Presented Papers

- Quantum Reinforcement Learning for Semantic Ranking of Enzyme Functionality, American Physical Society, Murat Isik and Sabre Kais, March 2026
- Enzyme Sequence Function Annotation Using Transformer for Discovery of Novel Biocatalysts, College of Engineering Networking Gatherings at Purdue University, Murat Isik and Sabre Kais, April 2025
- Quantum Machine Learning for Enzyme Function Prediction, Stanford Quantum Science Symposium, Murat Isik, and Sabre Kais, September 2025
- Multimodal Quantum Vision Transformer for Enzyme Commission Classification from Biochemical Representations, IEEE International Conference on Quantum Artificial Intelligence, Murat Isik and Sabre Kais, November 2025
- Quantum energy teleportation: A novel protocol relaxing previous constraints, APS Global Physics Summit 2025
Songbo Xie and Sabre Kais, 03/21/2025 (Contributed Talk)
- Modulator-Assisted Local Control of Quantum Battery via Zeno Effect, Rochester Conference on Coherence and Quantum Science 2025, Songbo Xie and Sabre Kais, 06/23/2025 (Contributed talk)
- Modulator-Assisted Indirect Control of Quantum Battery via Zeno Effect, QC-HORIZON 2025 Proceedings
Songbo Xie and Sabre Kais, 08/26/2025 (Keynote session. Joint presentation with Prof. Sabre Kais)
- Modulator Assisted Indirect Control of Quantum Battery via Zeno Effect, Battery and Energy Storage Symposium
Songbo Xie, and Sabre Kais. 01/20/2026 (Poster, People's Choice Poster Award)
- Chiral Discrimination on Gate-Based Quantum Computers, Photochemistry Symposium (NC Photochem), Muhammad Arsalan Ali Akbar and Sabre Kais, November 8, 2025
- Digital quantum simulation of wavepacket correlations in a chemical reaction, NC PhotoChem 2025, Shah Ishmam Mohtashim and Sabre Kais, November 8, 2025
- A hybrid quantum-classical algorithm for computing Scattering Matrix Elements, Quantum Information Processing Conference 2025, Shah Ishmam Mohtashim and Sabre Kais, February 25, 2025

- Disordered Phases in Quantum Circuit Simulations of the Ising Model Hint at Glassy Dynamics, Noise and Decoherence in Qubits, Shah Ishmam Mohtashim and Sabre Kais, February 25–March 1, 2024
- APS March Meeting 2023 March 5–10, 2023 | Las Vegas, Nevada, “Comparison of Random Circuit Sampling on Quantum and Classical Processors”, S. Oh and S. Kais
- APS March Meeting 2023 March 5–10, 2023 | Handling Privacy-sensitive Clinical Data with Federated Quantum Machine Learning A Bhatia, S Kais, M Alam
- APS March Meeting 2023 March 5–10, 2023 | Psitrum and Simulation of Decoherence in Quantum Algorithms M Alghadeer, S Kais, F Alharbi
- APS March Meeting 2023 March 5–10, 2023 | Demystifying a generative Quantum Machine Learning model using Information scrambling and Imaginary components of out-of-time correlators. M Sajjan, V Singh, S Kais
- APS March Meeting 2023 March 5–10, 2023 | Using Quantum Circuits with Convolutional Neural Networks for Multi-Object Detection and Classification M Saggi, S Kais
- APS March Meeting 2022 Monday–Friday, March 14–18, 2022; Chicago Session K40: Noisy Intermediate Scale Quantum Computers VI, “Non-Randomness of Google's Quantum Supremacy Benchmark”, Sangchul Oh and Sabre Kais, Purdue University.
- APS March Meeting 2022 Monday–Friday, March 14–18, 2022; Chicago, “Statistical Correlation Between Quantum Entanglement and Spin–Orbit Coupling in Crossed Beam Molecular Dynamics”, Sumit Suresh Kale, Junxu Li, Manas Sajjan and Sabre Kais
- APS March Meeting 2022 Monday–Friday, March 14–18, 2022; Chicago, scaling Up Quantum Characterization and Validation, Convergence of a reconstructed Density Matrix to a Pure State using the Maximal Entropy Approach”, Rishabh Gupta, Raphael Levine and Sabre Kais
- APS March Meeting 2022 Monday–Friday, March 14–18, 2022; Chicago, “Statistical Approach to Quantum Phase Estimation”, Yuchen Wang, Alexandria Moore, Zixuan Hu, Sabre Kais, Andrew M Weiner
- APS March Meeting 2022 Monday–Friday, March 14–18, 2022; Chicago, Quantum Digital and Analog Algorithms, “Finite-Size Scaling on a Digital Quantum Simulator using Quantum Restricted Boltzmann Machines”, Bilal Khalid, Shree Hari Sureshbabu, Arnab Banerjee, Sabre Kais.
- APS March Meeting 2022 Monday–Friday, March 14–18, 2022; Chicago, Quantum Dynamics, “Statistical Correlation Between Quantum Entanglement and Spin-Orbit Coupling in Crossed Beam Molecular Dynamics”, Sumit S Kale , Sumit S Kale, Sabre Kais and Junxu Li.
- Kais group members gave 7 talks at the APS March Meeting 2021.
- Solving Set Cover with Pairs with quantum annealing, Poster. Workshop on quantum control of light and matter. Purdue University, West Lafayette, IN. October, 2015 (with Yudong Cao)

- Efficient optimization of perturbative gadgets using cellular automata. Poster. NIST-UMD Workshop on Quantum Information and Computer Science (QuICCS). University of Maryland, College Park, MD. October, 2015. (With Yudong Cao)
- Perturbative reductions for quantum many-body Hamiltonians. Invited talk. Workshop on Novel Computing Approaches to Quantum Chemistry. Telluride, CO. July, 2015 (Yudong Cao)
- 1st International Solar Fuels Conference, April 26-May 1, 2015. Uppsala, Sweden "Quantum Dynamics of Biologically Inspired Photocells"
- QEERI International Computational Workshop on Solar Energy", April 11-14, 2015, Doha, Qatar "Revealing the role of organic cations in hybrid halide perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$ "
- QEERI International Computational Workshop on Solar Energy, April 11-14, 2015, Doha, Qatar, "Domain Walls Conductivity in Hybrid Organometallic Perovskites and Their Essential Role in $\text{CH}_3\text{NH}_3\text{PbI}_3$ Solar Cell High Performance"
- 39th Midwest Theoretical Chemistry Conference Indiana University, Bloomington, June 28-30, 2007."Quantum Algorithm for Obtaining the Energy Spectrum of Molecular System" (with Hefeng Wang)
- 39th Midwest Theoretical Chemistry Conference Indiana University, Bloomington, June 28-30, 2007."Finite Size Scaling and Gaussian Basis Sets" (with Winton Moy)
- 39th Midwest Theoretical Chemistry Conference Indiana University, Bloomington, June 28-30, 2007."Dimensional Scaling Treatment of Stability of Atomic and Anions Induced by Superintense Laser Fields" (with Qi Wei)
- 39th Midwest Theoretical Chemistry Conference Indiana University, Bloomington, June 28-30, 2007. "Entanglement Amplification by external Interactions" (with Zhen Huang)
- 39th Midwest Theoretical Chemistry Conference Indiana University, Bloomington, June 28-30, 2007."Entanglement and Quantum Phase Transitions" (with. Wang)
- Chair a session on Conductance in Molecules, The Fritz Haber Center, Hebrew University, June 11, 2007, and
- Chair of a session on Electron Dynamics, The Quantum World in Real Time: Is it Accessible?, Safed-Israel, June 25, 2007.
- APS March Meeting 2007, Denver, Colorado, March 5-9, 2007.Session W18: Theoretical Methods and Algorithms, with Hefeng Wang, ``Quantum Entanglement and Electron Correlation in Molecular Systems"
- APS March Meeting 2007, Denver, Colorado, March 5-9, 2007.Session K1: Poster Session II, with Hefeng Wang, ``Quantum Teleportation in One-Dimensional Quantum Dots System"
- Princeton-TAMU Foundations of Quantum Mechanics Symposium, Poster ``Finite Size Scaling in Quantum Mechanics", Princeton, 16-17 February 2007.\\"
- 3rd International Congress of Nanotechnology, San Francisco, ``Quantum Teleportation using Quantum Dots", with Hefeng Wang, November 2, 2006.
- 38th Midwest Chemistry Conference, "Finite Size Scaling in Quantum Chemistry", Ohio State University Campus, Columbus Ohio, June 15-17, 2006.

- Nanostructured materials and nanotechnology Symposium, IMRC2006.with Zhen Huang ``Entanglement Evolution under Fluctuation of external magnetic Field", August 22, 2006.
- International Congress of Nanobiotechnology and nanomedicine, Poster with Hefeng Wang, ``Quantum Teleportation in One-Dimensional Quantum Dots", San Francisco, June 19-21, 2006.
- NASA INAC Molecular Conductivity and Sensor Workshop, Purdue University, July 27-29, 2005.
- 37th Midwest Theoretical Chemistry Conference, June 16-18, 2005, University of Missouri-Columbia, MI, "Dephasing of Entanglement Under Fluctuation of External Magnetic Field", Zhen Huang and Sabre Kais.
- 37th Midwest Theoretical Chemistry Conference, June 16-18, 2005, University of Missouri-Columbia, MI
- "Finite Size Scaling with Gaussian Basis Set" Winton Moy and Sabre Kais. 37th Midwest Theoretical Chemistry Conference, June 16-18, 2005, University of Missouri-Columbia, MI "Entanglement and Quantum Phase Transition in 1D Hubbard Model with Impurity" Hefeng Wang and Sabre Kais.
- 37th Midwest Theoretical Chemistry Conference, June 16-18, 2005, University of Missouri-Columbia, MI "Tuning the Entanglement for 2D Array of Quantum Dots" David Lyvers and Sabre Kais. 37th Midwest Theoretical Chemistry Conference, June 16-18, 2005, University of Missouri-Columbia, MI "Finite Size Scaling for Quantum Critical Phenomena in a Laser Field "Qi Wei and Sabre Kais.
- Sanibel Symposium 2005 in Quantum Chemistry, Florida, March 5, 2005. "Tuning Entanglement for Magnetic Systems"
- 36th Midwest Theoretical Chemistry Conference, June 17-19, 2004 "Dynamics of Entanglement for One-Dimensional Spin Systems in an External Time-Dependent Magnetic Field" with Zhen Huang
- 36th Midwest Theoretical Chemistry Conference, June 17-19, 2004 "Finite Size Scaling for the Atomic Shannon Entropy", with Qicun Shi
- 36th Midwest Theoretical Chemistry Conference, June 17-19, 2004 "Metal-Insulator Transition and Entanglement for a 2D array of Quantum Dots", with David Lyvers
- Sanibel Symposium 2004 in Quantum Chemistry, Florida, February 28, 2004. "Finite Size Scaling for the Entanglement in an Itinerant Two-Dimensional Fermionic Systems"
- Fourth International Conference on Dynamic Systems and Applications May 21-24, 2003 Department of Mathematics, Morehouse College Atlanta, Georgia, USA, "Finite Size Scaling for Quantum Critical Phenomena and Stability of Atomic and Molecular Systems".
- Sanibel Symposium 2003 in Quantum Chemistry, Florida, February 23, 2003. "Finite Size Scaling in Quantum Mechanics"

- APS March Meeting 2003, March 3-7, Austin, Texas "Proposal for an entanglement switch using impurities in a 1D magnetic system," Session S19, (Focus Session: Quantum Information Science II)
- Quantum Information Science March 23-28, 2003, Ventura, CA, "Proposal for an entanglement switch using impurities in a 1D magnetic system,"
- 35th Midwest Theoretical Chemistry Conference, June 12-14th 2003, Iowa State University, Ames, IA "Quantum Phase Transitions and Stability of Atomic and Molecular Systems". "Tuning the Entanglement for a 1D Magnetic System with Anisotropic Coupling and Impurities"
- Ohio-Michigan Physics Conference on Quantum Computing, Michigan State University, April 11-12, 2003 "Tuning the Entanglement for a 1D Magnetic System with Anisotropic Coupling and Impurities"
- The 15th annual workshop on recent developments in electronic structure algorithms, May 17-19, 2003, University of Minnesota ,Minneapolis, Minnesota, "Quantum Phase Transitions and Stability of Atomic and Molecular Systems".
- Harvard University, Department of Chemistry, Cambridge, MA Sept.20-22, 2002, Attending "New Frontiers of Chemical Physics Symposium"
- 2002 American Conference on Theoretical Chemistry, Champion, PA, July 13th-18, 2002 "Finite Size Scaling for Extended Systems"
- 2002 International Conference on Computational Nanoscience and Nanotechnology, ICCN 2002, April 22-25, 2002 San Juan , Puerto Rico " Finite Size Scaling in Quantum Mechanics"
- APS March Meeting 2002, Indianapolis, IN, March 22, 2002 Session X26 (Ice: Surface Structure and Dynamics II)"Parallel Tempering Microcanonical Monte Carlo Study of Water Cluster"
- APS March Meeting 2002, Indianapolis, IN, March 19, 2002 Session G21 (Structural Phase Transition)"Phase Transitions and Stability of Three-Body Coulomb Systems"
- APS March Meeting 2002, Indianapolis, IN, March 18, 2002 Session B21 (Metal-Insulator Phase Transition II)"Study of MIT in pure and disordered Hubbard Model on triangular lattice with real-space renormalization-group method"
- Sanibel Symposium 2002 in Quantum Chemistry, Florida, February 23, 2002. "Poster: Finite Size Scaling for Quantum Dots"
- 34th Midwest Theoretical Chemistry Conference, October 5-6, 2001, Minneapolis, Minnesota. "Quantum Phase Transitions and Stability of Atomic and Molecular Systems".
- Molecular Quantum Mechanics, An International Conference in Honor of Prof. E.R. Davidson Seattle, WA, July 21-26, 2001. "Quantum Phase Transitions and Stability of Atomic and Molecular Systems".
- Quantum Applications Symposium, University of Michigan, Ann Arbor, MI, July 1-3, 2001.
- The 13th annual workshop on recent developments in electronic structure algorithms, Princeton University, Princeton NJ, June 15-18, 2001 "Quantum Phase Transitions and Stability of Atomic and Molecular Systems".

- Condensed Matter Brazilian Meeting (XXIV ENFMC) May 15-18, 2001, Brazil "Critical Phenomena in Atomic and Molecular Systems: Mapping to Classical Lattices", Talk (with R.A. Sauerwein)
- MOLEC 2000 Symposium, Hebrew University, Israel "Resonance States of Atomic Anions", Poster with A.V. Sergeev
- The 33rd Midwest Theoretical Chemistry Conference, May 25-27, 2000, University of Iowa, Talk (with R.A. Sauerwein) "Path Integral Approach to Critical Phenomena in Atomic and Molecular Systems" Talk (with P. Nigra)"A Study of the Correlation Between Intensive Properties and Finite Size Effects in Water Clusters", Poster (with Q. Shi)"Finite Size Scaling Method for Diatomic Molecules".
- VI Latin American Workshop on Nonlinear Phenomena, Huerta Grande, CÃ³rdoba, Argentina, October 12-16, 1999,"Finite Size Scaling In Quantum Mechanics", (with Pablo Serra).
- 32st Midwest Theoretical Chemistry Conference Department of Chemistry, University of Notre Dame, Indiana, May 20-22, 1999
- Chair of one session at the Conference. "Stability of Simple Molecular Systems in a Strong Magnetic Field, with Dr. Qicun Shi", and "Finite Size Scaling Method and Gaussian Basis Sets for Molecular Critical Parameters, (Poster), "Pivot Method for Global Optimization: A Study of Water Clusters (H₂O)_N with 2 < N < 33 ", with Pablo Nigra, (Poster).
- The American Physical Society - 1999 March Meeting Atlanta, Ga 20-27 March, 1999 Poster: Finite Size Scaling method for the Stability of Atomic and Molecular Ion. and Stability of one-electron bond in a strong magnetic field
- Sanibel Symposium in Quantum Chemistry Florida, February 27, 1999 Poster: Critical Charges for N-Electron Atoms: Stability of Atomic Negative Ions.
- The American Physical Society - 1998 March Meeting Los Angeles, CA 16-20 March, 1998Talk: Phase Transitions and Stability of Atomic and Molecular Negative Ions Poster: Critical Parameters for Few Electron Systems.
- Sanibel Symposium in Quantum Chemistry Florida, February 21-27, 1998Poster: Finite Size Scaling for Electronic Structure of Atoms and Molecules.
- Coupled Cluster Theory and Electron Correlation Workshop Cedar Key, Florida, June 15-19, 1997 Abstract: Finite Size Basis Set Scaling Anstaz for Atoms.
- Ninth Annual Conference on Recent Developments in Electronic Structure Methods Cornell University, Ithaca, NY, May 31-June 2, 1997Poster: Finite Size Basis Set Scaling Anstaz for Atoms.
- 30th Midwest Theoretical Chemistry Conference University of Illinois, Urbana-Champaign, May 22-24, 1997Poster: Symmetry Breaking and Stability of Binary Clusters (with Pablo Serra) Poster: Finite Size Basis Set Scaling for Helium Like Atoms (with Juan Pablo Neirotti and Pablo Serra).
- Sanibel Symposium in Quantum Chemistry Florida, March 1-7, 1997 Poster: Renormalization Group Approach for Electronic Excitations in Atoms.

- Eighth Annual Conference on New Methods in Electronic Structure Calculations University of Minnesota, Minneapolis, June 14-17, 1996Poster: Symmetry Breaking and Critical Phenomena for Electronic Structure at the Large-Dimension Limit.
- Sanibel Symposium in Quantum Chemistry Florida, February 24-March 2, 1996 Abstracts: Critical Phenomena for Electronic Structure of Atoms and Molecules.
- Molecular Quantum Mechanics: Methods and Applications University of Cambridge, England, 3-7 September 1995Poster: Charge Renormalization at the Large-D Limit for Electronic Structure Calculations.
- Northwestern University, XXVIII Midwest Theoretical Chemistry Conference Evanston, Illinois, May 11-13, 1995Poster: Charge Renormalization at the Large-D Limit for Electronic Structure Calculations.
- Sanibel Symposium in Quantum Chemistry Florida, February 25 - March 4, 1995Poster: Dimensional Renormalization for Electronic Structure Calculations.
- Seventh Conference on Superconductivity and Application, SUNY at Buffalo Buffalo, NY, September 7-9, 1994 Superconductivity and Applications.
- Gordon Research Conference, New Hampshire Brewster Academy, NH, July 17-July 22, 1994 Solid State Chemistry.
- Institute for Theoretical Atomic and Molecular Physics Cambridge, MA, May 17-19, 1991Hidden Crossings in Ion-Atom Collisions and in Other Nonadiabatic Transitions.