

## Curriculum Vita

### Sabre Kais

Department of Chemistry and  
Purdue Quantum Science and Engineering Institute  
Purdue University  
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#### EDUCATION AND PROFESSIONAL EXPERIENCE

- 2021-Present Professor of the Elmore Family School of Electrical and Computer Engineering
- 2002-Present Full Professor of Chemical Physics, Purdue
- 2010-Present Professor of Physics (Courtesy Appointment), Purdue
- 2005-Present Professor of Computer Sciences (Courtesy Appointment), Purdue
- 2014-2019 External Research Professor at Santa Fe Institute
- 2013-2016 Research Director of the Theory Group, Qatar Environment and Energy Research Institute (QEERI).
- 2010-2013 Director, NSF Center for Chemical Innovation: Phase I, Quantum Information for Quantum Chemistry
- 2009 Visiting Professor, Hebrew University, Jerusalem
- 2010 Visiting Professor, Technion, Haifa
- 2008 Visiting Scientist, Max Planck Institute for Physics of Complex Systems, Dresden
- 2005 Visiting Guggenheim Fellow, Department of Chemistry, Stanford University
- 2000-2001 Forchheimer Visiting Professor, Department of Chemistry, Hebrew University of Jerusalem
- 1999-2002 Associate Professor, Department of Chemistry, Purdue University
- 1994-1999 Assistant Professor, Department of Chemistry, Purdue University
- 1992 Visiting Scientist, Department of Chemistry, Cambridge University, England (with Prof. N.C. Handy)
- 1992 Visiting Scientist, Department of Chemistry, Oxford University, England (with Prof. M.S. Child)
- 1989-1994 Postdoctoral Associate, Department of Chemistry Harvard University (with Prof. Dudley R. Herschbach)
- 1984-1989 Ph.D Theoretical Chemistry, Hebrew University of Jerusalem  
Adviser: Professor R.D. Levine and M. Cohen  
Thesis Topic: An Algebraic Approach to Calculate Atomic and Molecular Properties
- 1983-1984 M. Sc. Theoretical Chemistry, Hebrew University of Jerusalem  
Adviser: Professor M. Cohen  
Thesis Topic: Atoms in Strong Magnetic Fields: Perturbation Theory Approach
- 1979-1983 B. Sc. Chemistry, Hebrew University of Jerusalem

## AWARDS

- 2019 Herbert Newby McCoy Award  
The most prestigious award given by Purdue University in natural sciences.
- 2012 Sigma Xi Research Award, Purdue University
- 2007 Fellow of the American Association for the Advancement of Science  
'For Outstanding creative contribution to theoretical chemistry, particularly the development of a finite size scaling approach to calculate quantum critical parameters for atomic, molecular and quantum dot systems'
- 2006 Fellow of the American Physical Society  
'For the development of a finite size scaling approach to calculate quantum critical parameters for atomic, molecular and quantum dot systems'
- 2005 Guggenheim Fellowship Award, 2005  
'Studies in finite size scaling theory'
- 2004-2009 Purdue University Faculty Scholar
- 2000 Forchheimer Fellowship
- 1998 National Science Foundation - CAREER
- 1985 Landau Prize, Hebrew University of Jerusalem
- 1983 Farkash Prize, Hebrew University of Jerusalem

## PROFESSIONAL ACTIVITIES

**Editorial Board:** 2008-Present: Molecular Physics; 2009-Present: Interdisciplinary Sciences: Computational Life Sciences; Electronic Journal of Mathematical and Physical Sciences; and 2010-Present: Papers in Physics, 2013-present, Frontiers in Chemistry and Physics and Scientific Reports.

**Referee:** Physical Review Letters, Nature, Physical Review A, Physical Review B, Physical Review E, Journal of Chemical Physics, Chemical Physics Letters, Journal of Physical Chemistry, International Journal of Quantum Chemistry, Molecular Physics, Chemical Communications, American Journal of Physics, Physics letters A, International Journal of Quantum Information, Physical Chemistry Chemical Physics and Nature Communications.

**Reviewer:** The National Science Foundation, The Petroleum Research Fund of the American Chemical Society, Army Research Office, Department of Energy and Qatar Foundation.

**Organizer and Chair:** Quantum Machine Learning and Data Analytics Workshop at Purdue, September 5 - 6, 2019. ACS Levine's 80<sup>th</sup> birthday symposium, Boston August 19, 2018.; Invited session on "Near term applications of small scale quantum

computing, APS March Meeting (2017); QEERI International Computational Workshop on Solar Energy, April, 2015; The 7th Winter School on Quantum Information Science, February 2013 National Cheng Kung University; and Tutorial on Quantum Information and Computation for Quantum Chemistry, APS, March Meeting 2013; Banff workshop on Quantum Information for Quantum Chemistry, June 2011, Banff Canada; Winter School in Quantum Information for Quantum Chemistry, January 2012 Indian Wells, CA; Chair of the Midwest Theoretical Chemistry Conference, Purdue (2010); Chair of the Midwest Theoretical Chemistry Conference, Purdue (1998); Chair of 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, June 25, 2007 and Chair of Plenary Session on Multi-Scale Simulations Sanibel 2002.

## **MEMBERSHIPS IN PROFESSIONAL SOCIETIES**

- American Chemical Society
- American Physical Society
- American Association for the Advancement of Science
- Sigma Xi Society

## **PERSONNEL**

### **Graduate Students**

- Shree Hari Sureshbabu (ECE ) 2020-present (Quantum Machine Learning)
- Blake Wilson (ECE ) 2020-present (Quantum Machine Learning)
- Bilal Khalid (Physics) 2020-present (Quantum Topological Phase Transitions)
- Raja Selvarajan (Physics) 2017-present (Quantum Algorithms)
- Sumit Kale (Chemistry) 2019-present (Quantum Computing)
- Rishabh Gupta (Chemistry) 2019-present (Quantum Computing)
- Junxu Li (Physics) 2018-present (Quantum Machine Learning)
- Shuxian Jiang (Computer Science) 2012-2017 (Quantum Annealing)
- Yuchen Wang (Physics) 2017-Present (Quantum Entanglement)
- Rongxin Xia (Physics) 2016-2020 (Quantum Computing)
- Teng Bian (Physics) 2016-2020 (Quantum Information)
- Zhanfu Yang (Computer Science) 2018-2019 M.Sc (Quantum Machine Learning)
- Vineet Mohanty (Mechanical Engineering) 2017-Present (Quantum Phases)
- Yudong Cao (Computer Science) 2012-2016 (Quantum Algorithms)
- Rishabh Chandra (Mechanical Engineering) 2012-2014 (Quantum Algorithms)
- Cyrus Vandrevala (Physics) 2011-2014 (Entanglement in Materials)
- Yiteng Zhang (Physics) 2011-2016 (Entanglement in Biological Systems)
- Shu-Hao Yeh (Chemistry) 2010-2015 (Quantum Coherence in Photosynthesis)
- Edwin Antillon (Physics), 2009-2012 (Finite Size Scaling, Conformal Invariance)

- Anmer Deskin (Computer Science), 2009-2013 (Quantum Compiler)
- Ross Hellen (Chemistry) 2009-2014 (Dimensional Scaling)
- Jing Zhu (Chemistry) 2006-2012 (Quantum Algorithms for Global Optimization)
- Qi Wei (Chemistry) 2004-2010 (Dimensional Scaling and Stability of Matter)
- Hefeng Wang (Chemistry) 2004-2008 (Quantum Algorithms )
- Winton Moy (Chemistry) 2004-2010 (Finite Size Scaling and Finite Elements)
- Xu Qing (Physics) 2005-2010 (Finite Size Scaling for Spin Systems)
- Zheng Huang (Chemistry) 2002-2007 (Entanglement for Quantum Systems )
- Aaron Stanton (Chemistry) 1995-1999 (Pivot Methods for Global Optimization)
- Pablo Nigra (Chemistry) 1996-2001 (Pivot Methods for Global Optimization: A Study of Structures and Phase Changes in Water Clusters)
- Stephen Belair (Chemistry) 1998-2004 (Pivot Methods for the Solution of Schrodinger equation for Electronic Structure Problems)
- Imad Ladadwa (Physics) 1999- visiting student for 6 months, Department of Physics, University of Bergen, Norway (Finite Size Scaling for Quantum Scattering Theory)

### **Postdoctoral Associates**

- Dr. Richard Bleil, 1994-1995 (Professor of Chemistry at Dakota State University, Madison, SD)
- Dr. Pablo Serra, 1995-1997 (Professor of Physics at the University of Cordoba, Argentina)
- Dr. Juan Pablo Neirotti, 1997-1998 (Professor of Physics at Cidade University, Sao Paulo, Brazil)
- Dr. Alexei V. Seregeev, 1998-1999 (Research Assistant at the Chemistry Department, Ben Goroun University, Israel)
- Dr. Ricardo Sauerwein, Sept. 1999- 2001 (Professor of Physics at The University of Federal De Santa Maria, Brazil)
- Dr. Qicun Shi, 1998-2005 (Research Scientist at the Institute for Medical Engineering and Science, Cambridge)
- Dr. Jiexiang Wang, 2001-2004 (Professor of Physics, East China Normal University, China)
- Dr. Omar Osenda, May 2002-2004 (Professor of Physics at the University of Cordoba, Argentina )
- Dr. Felipe Herrera, April 2012-present (Assistant Professor of physics, Universidad de Santiago de Chile, Chile)
- Dr. Dong Wang, January 2014-January 2015 (Assistant Professor, School of Physics and Material Science, Anhui University, Hefei 230601, China)
- Dr. Sachin D. Yeole December 2014-2015 (Finite Size Scaling)
- Dr. Jiang Wang, August 2015-2016 (Professor Hefei, Quantum Computing)
- Dr. Nan Jiang, August 2015-2016 (Professor Hefei, Quantum Entanglement and Computing)
- Dr. Merid Legesse Belayneh, 2015-2017 (Quantum Materials for Solar Energy)
- Dr. Zixuan Hu, 2016-Present (Quantum Coherence and Computing )

- Dr. Shuhao Yeh, 2016-2019 (Quantum Coherence for Quantum Devices)
- Dr. Kumar Ghosh, 2018-2020 (Quantum Machine Learning)
- Dr. Vivek Dixit, 2019-2021 (Quantum Machine Learning )
- Dr. Yijue Ding 2018-2020 (Quantum Entanglement )
- Dr. Manas Sajjan 2020-Present (Quantum Transport and Quantum Computing)
- Dr. Sangchul Oh, 2020-Present (Quantum Algorithms)

## PROPOSALS FUNDED

- A New Approach to Global Minimization, ACS-PRF, \$20,000 6/1/96 - 8/31/98, PI: Sabre Kais
- Renormalization Group Approach for the Treatment of Electron Correlation, PRF, \$5,000 7/1/96 - 6/30/97, PI: Sabre Kais
- Critical Phenomena and Renormalization Group Approach for Electronic Structure Calculations ONR \$300,000 12/1/96 - 9/30/99 PI: Sabre Kais
- Scaling Theory for Electronic Structure NSF-CAREER \$340,000 10/15/98 - 4/15/2002 PI: Sabre Kais
- Critical Phenomena and Renormalization Group Approach for Electronic Structure Calculations ONR \$300,000 12/1/99 - 9/30/2002 PI: Sabre Kais
- Finite Size Scaling and Stability of Atomic and Molecular Ions ACS-PRF \$80,000 4/1/02 - 8/31/04 PI: Sabre Kais
- Critical Phenomena and Renormalization Group Approach for Electronic Structure Calculations ONR \$100,000 9/30/2002-12/1/2004 PI: Sabre Kais
- Scaling Theory for Electronic Structure, NSF \$291,000 2/1/02 - 01/31/06 PI: Sabre Kais
- Dynamics of Entanglement and Decoherence for Quantum Computing 2005 PRF \$13,776 7/1/05-6/30/06, PI Sabre Kais}
- Entanglement Production by Electron Transfer Processes in Mesoscopic and Molecular Systems, BNSF \$120,000 7/1/05-6/30/10, PI: Sabre Kais and Uri Peskin
- Stability of Multiply Charged Ions by Superintense Laser Fields 2007 PRF \$15,292 6/1/06-5/31/07, PI: Sabre Kais
- CPATH CB: Computing Education in Science Context, NSF \$446,000 7/1/07 - 6/30/10, Co-PI: Sabre Kais
- Quantum Phase Transitions for Atoms, Molecules and Quantum Degenerate Gases ARO \$100,000 7/1/07 - 6/30/08 PI: Sabre Kais
- Simulated Quantum Computation of Global Optimization 2008 PRF \$16,300 6/1/08-5/31/09, PI: Sabre Kais
- Finite Size Scaling and Quantum Criticality of Quantum Gases, ARO \$300,000 1/1/09 - 12/30/12, PI: Sabre Kais
- Quantum Computer Algorithm for Chemistry, 2009 PRF \$16,300 6/1/09-5/31/10, PI: Sabre Kais

- National Science Foundation Centers for Chemical Innovation, Phase I: Quantum Information and Computation for Chemistry, NSF, \$1,500,000, 10/1/2010-9/30/2013, PI Sabre Kais-Purdue, Co-PI's Alan Aspuru Guzik (Harvard), Ken Brown (Georgia Tech), Daniel Lidar (USC) and Peter Love (Haverford)
- Radical Chemistry on Cloud and Aerosol Surfaces, NSF \$775,000, 09/1/13 - 08/31/2015, PI Joseph Francisco, Co-PI Sabre Kais
- New chemistries for the catalytic conversion of natural gas to valuable organics Qatar Foundation, \$ 1,000,000 Oct. 1, 2013 -Sept 30, 2015, PI Mahdi Abu Omar, Co-PI Sabre Kais
- Quantum Aspects of the Non-adiabatic Electronic Energy Transfer Ignited by Sunlight in Photosynthetic Light-Harvesting Complexes, Purdue University Universidad de Antioquia Seed Grant Program, Sabre Kais (Chemistry, Purdue, \$6000) and Leonardo A. Pachon (Institute of Physics, Universidad de Antioquia, \$50,000), 2015-2017 .
- Studies of the role of electron correlations in potential-matched direct nonequilibrium solar refrigeration" Qatar Foundation, \$ 900,000 Oct. 1, 2014 - Sept. 30, 2017, PI Sabre Kais, Co-PI Fahhad Alharbi (QEERI) and Tim Fisher (Purdue)
- COHERENT ENERGY TRANSFER IN NOVEL EXCITONIC MATERIALS FOR SOLAR ENERGY APPLICATIONS, Qatar Foundation, \$ 5,000,000 for 5 years, starting January 31, 2016, PI Sabre Kais , Co-PI Fahhad Alharbi (QEERI) and Greg Engel (U Chicago).
- Quantum Machine Learning for Data Analytics and Optimization, \$300,000, 8/1/2018-8/1/2020, Discovery Park, Purdue Sabre Kais (PI), Yong Chen, Alex Pothén and Ashraf Alam (Co-PIs)

### **Current Grants:**

- DOE, "Quantum Computing Algorithms and Applications for Coherent and Strongly Correlated Chemical Systems \$2,475,000 09/15/2018 - 09/14/2021 Sabre Kais (PI), D. Mazziotti, Y. Chen L. Huang and J. Anderson (Co-PIs)

### **Renewed for additional 3 years \$3,000,000**

Sabre Kais (PI), D. Mazziotti, Prineha Narang, Y. Chen L. Huang and J. Anderson (Co-PIs)

- NSF RAISE-TAQS: High Dimensional Frequency Bin Entanglement - Photonic Integration and Algorithms." \$1,000,000 08/15/2018- 08/14/2021 Co-PI Sabre Kais , PI Andrew Weiner and Co-PI Minghao Qi (EEC-Purdue). NCE until 2022.

- Soar Technology, Inc., “Resisting Adversarial Attacks with Quantum Machine Learning”, \$45,000 04/01/2019 - 01/04/2020, Sabre Kais (PI).  
We got a letter of “Recommendation for Funding Letter” from DARPA for \$150,000 for one additional year.
- NSF, “Near Term Applications of Quantum Machine Learning Techniques to Quantum Chemistry”. \$450,000 09/1/2020- 08/31/2023, Sabre Kais (PI).
- ORNL, Quantum Science Center, DOE Center, \$115 Mil for 5 years. My grant “Developing quantum algorithms and quantum machine learning for materials”, \$750,000 , 1/9/2020- 8/31/2025 , Sabre Kais (PI).
- Air Force, “Quantum Machine Learning for Extended Systems”, \$75,000 , 9/1/202- 8/31/2021, Sabre Kais (PI). NCE until 2022.
- ORNL, Developing quantum machine learning methods for computational chemistry, supporting ½ postdoc position. \$50,000 9/1/2020- 8/31/2021, Sabre Kais (PI)
- PRF, “Quantum Machine Learning for Classifying Entanglement in Complex Systems”, Graduate School for 2020-21, this is estimated as \$20,782 in graduate salary and fringes, Sabre Kais (PI)
- Purdue Quantum Science and Engineering Institute, Seed Project , “Cryptography by image reconstruction using a quantum annealer, \$10,000 for the summer 2020, Sabre Kais (PI).
- CCI Phase I: NSF Center for Quantum Dynamics on Modular Quantum Devices (CQD-MQD), 1,800,000 09/01/2021 - 08/31/2024, Victor Batista (Yale , PI) Subawardees: Purdue University (Sabre Kais Co-PI \$330,000 ) University of Michigan ( Eitan Geva CO-PI) and Yeshiva University (Lea F. Santos Co-PI).
- NSF IUCRC Planning Grant Purdue University: Center for Quantum Technologies (CQT), \$20,000 6/1/2021-12/30/2021, Sabre Kais (Center Director, PI), Collaborations: Purdue, IU, ND and IUPUI

## RESEARCH PROGRAM

The research in our group is mainly devoted to treat the following problems:

- **Quantum Algorithms**

In the area of quantum algorithms for quantum chemistry, Prof. Kais has made significant progress on elucidating, optimizing and implementing ground state algorithms, in particular electronic structure problems on quantum computers. He has also developed methods based on quantum algorithms for solving linear equations, specifically Poisson's equation. He has found orders of magnitude improvement in the length of the algorithm (circuit depth) by finding more efficient ways to emulate the wavefunction evolution on a quantum computer. See for example, the following papers: *J. Phys. Chem. B*, 122, 3384-3395 (2018); *Quantum Information & Computation*, 17, 9-10, 779-809 (2017); *Quantum Information Processing*, 16:1 DOI: 10.1007/s11128-016-1452-3 (2017); *Quantum Information Processing*, 14, 891-899 (2015); *Journal of Chemical Physics*, 141, 224108 (2014); *Physical Review A*, 89, 022313 (2014); *Quantum Information Processing*, 13, 333-353 (2014); *New Journal of Physics*, 15, 013021 (2013), *Journal of Chemical Physics*, 137, 234112 (2012) and *Scientific Reports* 8:17667 (2018)

- **Quantum Machine Learning**

Quantum machine learning — a hybridization of classical machine learning techniques with quantum computation — is emerging as a powerful strategy for improving the efficiency of both quantum classical machine learning algorithms. Prof. Kais has developed a hybrid quantum algorithm employing a restricted Boltzmann machine to obtain accurate molecular potential energy surfaces. By exploiting a quantum algorithm to help optimize the underlying objective function, Prof. Kais obtained an efficient procedure for the calculation of the electronic ground state energy for a small molecule system. This approach achieves high accuracy for the ground state energy of simple molecular systems at a specific location on its potential energy surface with a finite basis set. With the future availability of larger-scale quantum computers, quantum machine learning techniques are set to become powerful tools to obtain accurate values for electronic structures. See, for example, *Nature Communications*, 9, 4195 (2018).

- **Quantum Coherence**

Prof. Kais developed a new quantum formalism to understand the role of quantum coherence in complex systems and used this strategy to prove that the efficiency of photocell is greatly enhanced by quantum coherence. Remarkably, in plants, bacteria and algae, the photon-to-charge conversion efficiency is about 100% under certain conditions. This fact is of great interest in understanding how nature



has achieved such high photovoltaic conversion efficiency by optimizing molecular processes such as trapping, radiative, and non-radiative losses, and particularly the role of quantum coherence to enhance transport in photosynthesis. Kais developed a new quantum formalism to understand the role of coherence in such systems. To do so he considered a linearly-aligned system as a light-harvesting antennae composed of two-level optical emitters coupled with each other by dipole–dipole interactions. Due to cooperative effects he found that certain dark states can enhance intra-band phononic dissipation to increase output power when incorporating more emitters in the linear system. These results suggest a promising novel design aspect of photosynthesis-mimicking photovoltaic devices, as described in the following manuscripts: *Proceedings of the National Academy of Science (PNAS, Latest Articles)*, DOI:10.1073/1701390115 (2018); *Frontiers in Physics*, 6,25 (2018); *The Journal of Chemical Physics*, 148, 064304 (2018); *Chem*, 4, 139-149 (2018); *Proceedings of the National Academy* 114, 22 5595-5600 (2017); *Scientific Reports*, 6, 30305 (2016); *Phys. Chem. Chem. Phys.*, (PCCP) 18, 31845 (2016); *Phys. Chem. Chem. Phys P* 17, 5743-5750 (2015); *Renewable & Sustainable Energy Reviews*, 43, 1073-1089 (2015); *International Journal of Quantum Chemistry*, 115, 15 (2015); *Physical Review E*, 87, 062704 (2013)).

- **Dimensional Scaling and Finite Size Scaling for Quantum Phase Transitions and Critical Phenomena:** We have established an analogy between symmetry breaking of electronic structure configurations and quantum phase transitions at the large dimensional limit. Furthermore, we have developed the finite size scaling method for quantum systems. In this case, the finite size corresponds not to the spatial dimension but to the number of elements in a complete basis set used to expand the exact wave function of a given Hamiltonian.

## TEACHING

For over 25 years, I have taught many undergraduate and graduate courses in chemistry, physics and math for science and engineering students. The list includes physical chemistry for chemists, science and engineering students, modern physics, introduction to chemical bond, statistical mechanics for chemistry students, statistical physics, introduction to quantum mechanics, advanced quantum mechanics, quantum chemistry, computational methods, advance math, quantum information and computation, global optimization, density functional theory and advanced special topics in material science, chemistry and physics.

## 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 Morse 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, 3990-3998 (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. Germann 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. Germann, and D.R. Herschbach, Large-Dimension Limit Yields Generic Potential Curves for H<sub>2</sub><sup>+</sup>, H<sub>2</sub>, HHe<sup>+</sup>, and He<sub>2</sub><sup>++</sup>, *J. Phys. Chem.* 98, 11015-11017 (1994).
  26. R. Bleil, F.M. Tao and S. Kais, Structure and Stability of C<sub>13</sub> Carbon Clusters, *Chem. Phys. Lett.* 229, 491-294 (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 Nb<sub>6</sub>C<sub>70</sub><sup>+</sup>, *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).
  37. P. Serra. A.F. Stanton and S. Kais, Pivot Method for Global Optimization, *Phys. Rev. E* 55, 1162-1165 (1997).
  38. P. Serra and S. Kais, Mean Field Phase Diagrams for One-Electron Molecules, *J. Phys. A* 30, 1483-1493 (1997).

39. P. Serra, A.F. Stanton, S. Kais and R. Bleil, Comparison Study of Pivot Methods for Global Optimization, *J. Chem. Phys.* 106, 7170-7177 (1997).
40. N.H. March and S. Kais, "Kinetic Energy Functional Derivative for the Thomas-Fermi Atom in D-Dimensions", *Int. J. Quantum Chem.* 65, 411-413 (1997).
41. Pablo Serra and Sabre Kais, "Symmetry Breaking and Stability of Binary Clusters", *Chem. Phys. Letters* 275, 211-214 (1997).
42. Juan Pablo Neirotti, Pablo Serra and Sabre Kais, "Electronic Structure Critical Parameters from Finite-Size Scaling", *Phys. Rev. Lett.* 79, 3142-3145 (1997).
43. Q. Chen, H. Chen, S. Kais and B.S. Freiser, "Gas-Phase Reactions of  $\text{Fe}(\text{CH}_2\text{O})^+$  and  $\text{Fe}(\text{CH}_2\text{S})^+$  with Small Alkanes: An Experimental and Theoretical Study", *J. Am. Chem. Soc.* 119, 12879-12888 (1997).
44. P. Serra, J.P. Neirotti and S. Kais, "Critical Parameters for the Helium-like atoms: A Phenomenological renormalization study", *J. Chem. Phys.* 108, 2765-2770 (1998).
45. 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.
46. P. Serra, J. P. Neirotti and S. Kais, "Finite-Size Scaling Approach for the Schrodinger Equation", *Phys. Rev. A. Rapid Communications*, 57, R1481-1484 (1998).
47. G. Murthy and S. Kais, "Renormalization Group Approach for Electronic Excitations in Atoms", *Chem. Phys. Lett.* 290, 199-204 (1998).
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  200. Rongxin Xia, Teng Bian, Sabre Kais, Electronic Structure Calculations and the Ising Machine, submitted *Nature Chemistry* (2016).
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241. Zixuan Hu, Rongxin Xia, Sabre Kais, "Quantum Algorithm for Evolving Open Quantum Dynamics on Quantum Computing Devices", *Sci Rep* 10, 3301 <https://doi.org/10.1038/s41598-020-60321-x> (2020).
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243. Xia, Rongxia; Kais, Sabre , "Hybrid Quantum-Classical Neural Network for Calculating Ground State Energies of Molecules, *Entropy*, Vol 11, 8, DOI 10.3390/e22080828 (2020).
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245. Xia, Rongxia; Kais, Sabre, "Qubit Coupled Cluster Singles and Doubles Variational Quantum Eigensolver Ansatz for Electronic Structure Calculations", *Quantum Sci. Technol.* 6, 015001, DOI.org/10.1088/2058-9565/abbc74 (2021)
246. Wang, Yuchen; Hu, Zixuan; Sanders, Barry and Kais, Sabre , "Qudits and High-Dimensional Quantum Computing, *Frontiers in Physics*, 8, 589504, DOI:10.3389/fphy.2020.589504 (2020).
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248. Szczesniak, Dominik; Kais, Sabre, "Magnetic Flux Noise in Superconducting Qubits and the Gap States Continuum", *Nature.com/ Scientific Reports*, DOI 10.1038/s41598-021-81450 (2021).



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250. Brian S. Rolczynski, Shu-Hao Yeh, Polina Navotnaya, Lawson T. Lloyd, Alan R. Ginzburg, Haibin Zheng, Marco A. Allodi, John P. Otto, Khuram Ashraf, Alastair T. Gardiner, Richard J. Cogdell, Sabre Kais, and Gregory S. Engel, “Time-Domain Line-Shape Analysis from 2D Spectroscopy to Precisely Determine Hamiltonian Parameters for a Photosynthetic Complex”, DOI: 10.1021/acs.jpcc.0c08012, The Journal of Physical Chemistry B 125, 2812-2820 (2021)
251. Rishabh Gupta, Raphael D. Levine and Sabre Kais , “Convergence of a Reconstructed Density Matrix to a Pure State Using the Maximal Entropy Approach”, J. Phys. Chem. A DOI: 10.1021/acs.jpca.1c05884 (2021).
252. Sureshbabu, Shree Hari; Sajjan, Manas; Oh, Sangchul; Kais, Sabre, “Implementation of Quantum Machine Learning for Electronic Structure Calculations of Periodic Systems on Quantum Computing Devices”, J. Chem. Inf. 61, 2667-2674 (2021).
253. Vivek Dixit, Raja Selvarajan, Muhammad A. Alam, Travis S. Humble and Sabre Kais, “Training Restricted Boltzmann Machines with a D-Wave Quantum Annealer”, Front. Phys. 9:589626. DOI: 10.3389/fphy.2021.589626 (2021).
254. Junxu Li, Zixuan Hu, and Sabre Kais, “Practical quantum encryption protocol with varying encryption configurations” PHYSICAL REVIEW RESEARCH 3, 023251 (2021) DOI: 10.1103/PhysRevResearch.3.023251 (2021).
255. Bian, Teng; Kais, Sabre, “Quantum Computing for Atomic and Molecular Resonances”, J. Chem. Phys. 154, 194107, doi.org?10.1063/5.0040477 (2021).
256. Dixit, Vivek; Selvarajan, Raja; Kais, Sabre, “Training a Quantum Annealing Based Restricted Boltzmann Machine on Cybersecurity Data” IEEE Transactions on Emerging Topics in Computational Intelligence, 10.1109/TETCI.2021.3074916 (2021).
257. Roy, Sayan; Hu, Zixuan; Bermel, Peter; Kais, Sabre , “Enhancement of Photovoltaic Current through Dark States in Donor-Acceptor Pairs of Tungsten-Based Transition Metal Di-Chalcogenides” Advanced Functional Materials 2100387, DOI: 10.1002/adfm.202100387 (2021).
258. Junxu Li and Sabre Kais, “A universal quantum circuit design for periodical functions”, New J. Phys. 23 103022, DOI: 10.1088/1367-2630/ac2cb4 (2021)
259. Junxu Li, Manas Sajjan, Sumit Suresh Kale, and Sabre Kais, “Statistical Correlation Between Quantum Entanglement and Spin–Orbit Coupling in Crossed Beam Molecular Dynamics”, Adv. Quantum Technol. 2100098. DOI: 10.1002/qute.202100098 (2021).

## 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, "Quantum Machine Learning for Complex Chemical Systems", Invited by **Chemical Society Reviews** (IF 54.6), in progress (2021).

## 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/ePhgE3Q> 2021.

## Invited Lectures

1. MIT, Physical Chemistry Seminar, Quantum information and quantum computing for complex systems", November 2, 2021.
2. Virtual Learning University, Morocco, Quantum information and quantum computing for complex systems", October 16, 2021.
3. The Solemn plenary session on "Quantum Computing", February 22-24, 2022, of The Hassan II Academy of Science and Technology, Morocco.
4. Boeing, "Quantum Machine Learning for Complex Systems", Wednesday, September 22, 2021
5. IBM Qiskit Series, Quantum Machine Learning for Complex Chemical Systems", Friday August 27, 2021.
6. 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.
7. ONLINE Lorentz-CECAM workshop 'Useful Quantum Computing for Quantum Chemistry' (22-26 February 2021), Quantum Algorithms for Evolving Open Quantum Dynamics, Feb. 25<sup>th</sup>, 2021.

8. Purdue University, MacCoy Award Distinguished Lecture, Quantum Information and Quantum Computing for Complex Chemical Systems, October 28, 2019.
9. Harvard University, Department of Physics (Harvard Quantum Initiative) , “Quantum Machine Learning for Complex Systems”, November 6, 2019.
10. 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.
11. DOE PIs meeting, “Quantum Computing Algorithms and Applications for Complex Chemical Systems”, Gaithersburg Maryland, May 21-24, 2019.
12. Argonne National Lab, Quantum Information and Computation for Chemistry, Chicago, May 7, 2019.
13. Yale University , Quantum Information and Computation for Chemistry, , May 3, 2019.
14. International Symposium of Quantum Science and technology at Purdue, “Quantum Computing for Chemistry”, April 21-23, 2019.
15. Purdue-IU Quantum workshop, “Quantum Algorithms for Chemistry, Feb. 26, 2019.
16. The 59th Sanibel Symposium “Quantum Computing for Complex Chemical Systems” Quantum Theory Project, University of Florida, February 17 - 22, 2019.
17. 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.
18. NSF “Quantum Computing Workshop”, Nov. 7, 2018. Quantum Computing for chemistry.
19. NIST workshop on Complex Systems Chemistry, Gaithersburg, Maryland, “Quantum Information and Computing for Chemistry”, October 22-24, 2018.
20. National Academies of Sciences, Engineering & Medicine, Chemical Sciences Roundtable, “Quantum Computing”, Friday, July 27, 2018.
21. Israeli Academy of sciences, Quantum Machine Learning for Electronic Structure, June 18, 2018, Jerusalem.
22. Air Force Institute of Technology 2950 Hobson Way WPAFB OH, “Near term applications of small scale quantum computing for quantum chemistry”, May 3, 2018.
23. IBM-Zurich, “Near term applications of small scale quantum computing for quantum chemistry”, June 6, 2018.
24. "Cold molecules for chemistry" symposium at ACS Spring meeting, “Quantum computing with polar molecules”, March 18-20 2018.
25. NASA, Lockheed-Martin center for Innovation, Suffolk, VA, Near term applications of small scale quantum computing for quantum chemistry, November 7, 2017.

26. Department of Chemistry, University of Chicago, Near term applications of small scale quantum computer”, October 24, 2017.
27. 254<sup>th</sup> ACS Meeting, Mapping electronic structure Hamiltonian to an Ising type Hamiltonian , August 20-21, 2017.
28. Department of Physics, Purdue University, “Near term applications of small scale quantum computer”, April 27, 2017.
29. APS, March Meeting 2017, Charing the Session “Near term applications of small scale quantum Computing”, New Orleans, March 13-17, 2017.
30. Department of Computer Science, Purdue University, “Near term applications of small scale quantum computer”, February 27, 2017.
31. Department of Mathematics, Purdue University, “Near term applications of small scale quantum computer”, February 10, 2017.
32. Wabash College, Department of Physics, Crawfordsville, IN 47933, “Near term applications of quantum computing”, February 6, 2017.
33. Oak Ridge National Laboratory, Quantum Information and Computation: Second Quantum Technology Revolution, January 11, 2017.
34. Zurich IBM Research Laboratory, Adiabatic Quantum Computing, January 25, 2017.
35. 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.
36. Challenges of Electronic Structure Calculations on Quantum Computers, Department of Chemistry, Purdue University, November 16, 2016.
37. Freie Universität Berlin, Challenges of Electronic Structure calculations on Quantum Computers, October 4, 2016.
38. Department of Chemistry, University of Virginia, Quantum Information and Quantum Computation for Chemistry, September 30, 2016.
39. Department of Computer Engineering, Istanbul Medeniyet University, Kadikoy, Istanbul, Turkey, Light Matter Interaction: The role of quantum coherence, April 5, 2016.
40. Swiss Chemical Society, Fall Meeting 2015, Lausanne, Challenges of Electronic Structure Calculations, Sept. 4, 2015.
41. 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
42. KAUST, Saudi Arabia, "Light matter interactions", April 29, 2015.
43. Qatar Foundation, "New Challenges for Electronic Structure calculations", April 13, 2015.
44. Swiss Chemical Society, Fall Meeting 2014, Zurich, Light Matter Interaction, Sept. 11, 2014.
45. IBM Zurich, Switzerland, Challenges of Electronic Structure Calculations for Atoms and Molecules, Zurich, Switzerland, Feb. 26, 2014.
46. Laboratory of Physical Chemistry, ETH, Quantum Coherence and Light matter Interaction, ETH, Zurich, Switzerland, Feb. 27, 2014.

47. Physics and Engineering ICube Laboratory/CNRS, University of Strasbourg, Light Matter Interaction : The role of quantum coherence, Strasbourg, France, Feb. 24, 2014
48. State Key Laboratory of Precision Spectroscopy East China Normal University, Challenges of Electronic Structure Calculations for Atoms and Molecules", Shanghai, China Dec. 1, 2013.
49. China Academy of Engineering Physics, Light Matter Interaction, Mianyang, China Dec. 3, 2013
50. China Academy of Engineering Physics, The Role of Quantum Coherence in Different Systems , Mianyang, Dec. 4, 2013
51. Sigma Xi Award Lecture, Quantum Information for Quantum Chemistry, Purdue, March 25, 2013.
52. 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
53. APS March Meeting 2013, March 18 - March 22, Baltimore, Maryland Tutorial 4 Quantum Information and Computation for Quantum Chemistry.
54. Santa Fe Institute, Quantum Coherence and Entanglement in Complex Systems, April 6, 2012.
55. Los Alamos National Lab, Quantum Entanglement, April 5, 2012.
56. Quantum Computation for Quantum Chemistry: Status, Challenges, and Prospects, Microsoft Research Redmond, Nov, 12, 2012, Redmond, WA
57. Winter School 2012, Quantum Information and Computation for Quantum Chemistry, January 5-7, 2012 at Indian Wells, CA
  
58. Banff Meeting, BIRS workshop on Quantum Information for Quantum Chemistry, June 6-11, 2011, Banff, Canada.
59. 241st ACS meeting, Division of Physical Chemistry, Anaheim, CA, Tuning and Quenching Entanglement of Dipole Arrays, March 30, 2011
60. Computer Science Department, Purdue University, Quantum Information and Quantum Computation, March 9, 2011.
61. 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.
62. King Abdullah Institute for Nanotechnology, Riyadh, Saudi Arabia, Research Projects in Birck Nanotechnology Center at Purdue, December 20, 2010.
63. Department of Physics (Malaz), King Saud University, Riyadh, Saudi Arabia, Quantum Information and Quantum Computation: Toward Realizing a Quantum Computer, December, 21 2010.
64. Department of Physics, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia, Finite Size Scaling, December 25, 2010.
65. Department of Physics, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia, Quantum Information and Computation, December 26, 2010.

66. Department of Physics, East China Normal University, China, Finite Size Scaling and Quantum Criticality, November 25, 2010.
67. Chinese Academy of Engineering Physics, Mianyang, China, Stability of Atomic and Molecular Systems in Superintense Laser Fields, November 26, 2010.
68. Purdue University, Computer Science, "Quantum Information and Quantum Computation", October 6, 2010.
69. TMAU-Princeton Summer Workshop on Quantum Optics and Molecular Physics, Quantum Information for Quantum Chemistry\ Casper, Wyoming, July 25-31, 2010.
70. 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, 2010.
71. 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.
72. Chair: 42nd Midwest Theoretical Chemistry Conference, Department of Chemistry, Purdue, May 20-22, 2010.
73. Department of Physics, Purdue, Quantum Information for Quantum Chemistry", February 11, 2010.
74. The 41st Midwest Theoretical Chemistry Conference, "Finite Size Scaling and Quantum Criticality", Southern Illinois University, Carbondale Illinois, May 28-30, 2009.
75. Rutgers University, THE 101ST STATISTICAL MECHANICS CONFERENCE, "Finite Size Scaling in Quantum Mechanics", SUNDAY - TUESDAY, MAY 10-12, 2009.
76. 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.
77. Fritz Haber Institute of the Max Planck Society, Department of Molecular Physics, Berlin, Germany" Finite Size Scaling and Quantum Criticality", December 12, 2008.
78. Ruhr University, Institute for Theoretical Chemistry, Bochum, Germany" Finite Size Scaling and Quantum Criticality", December 3, 2008.
79. 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.
80. Technical University of Dresden, Department of Physics," Finite Size Scaling and Quantum Computing", November 13, 2008. Technical University of Munich, Institute for Measurement Systems and Sensor Technology, Munich, Germany," Finite Size Scaling and Quantum Computing", October 22, 2008.
81. University of Heidelberg, Institute for Theoretical Chemistry, Universitaet Heidelberg, Germany," Finite Size Scaling and Quantum Criticality", October 20, 2008.
82. Freie Universitaet Berlin, Department of Chemistry, Berlin, Germany" Finite Size Scaling in Quantum Mechanics", September 10, 2008.

83. Max Planck Institute for Physics of Complex Systems, Dresden, Germany "Quantum Criticality", August 22, 2008.
84. University of Chicago, James Franck Institute (JFI), "Suppose We Build a Quantum Computer, How Chemistry Can Benefit From Such a Computer", June 10, 2008.
85. Santa Fe Institute, "Finite Size Scaling and Quantum Criticality", February 7, 2008.
86. Harvard-MIT-BU-BC Theory Seminar, "Finite Size Scaling in Quantum Mechanics", November 26, 2007.
87. Purdue University, Electrical and Computer Engineering, Nano501 "Finite Size Scaling and Quantum Criticality", November 12, 2007.
88. Illinois Institute of Technology, Physical Sciences, "Finite Size Scaling for Atomic and Molecular Systems", October 25, 2007.
89. Illinois Institute of Technology, Chemical Engineering, "Quantum Phase Transition and Stability of Atomic and Molecular Systems", September 5, 2007
90. Technion-Israel, Department of Chemistry, "Finite Size Scaling in Quantum Mechanics", June 24, 2007.
91. Lewiner Institute of Theoretical Physics, Technion-Israel, Correlated Electrons Day, "Finite Size Scaling in Quantum Mechanics", June 21, 2007.
92. Yarmouk University, Jordan, "Quantum Phase Transition and Stability of Atomic and Molecular Systems", May 29, 2007.
93. 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"
94. Princeton-TAMU Foundations of Quantum Mechanics Symposium, "Dimensional Scaling for Stability of Atomic and Molecular Systems", Princeton, 16-17 February 2007.
95. Department of Chemistry, Purdue University, West Lafayette "Finite Size Scaling for Stability of Atomic and Molecular Systems", February 7, 2007.
96. 38th Midwest Chemistry Conference, "Entanglement and electron Correlation in Quantum Chemistry calculations", Ohio State University Campus, Columbus Ohio, June 15-17, 2006
97. The 36th Winter Colloquium on the Physics of Quantum Electronics, "Entanglement as a measure of electron-electron correlation", Snowbird, Utah, January 2-6, 2006.
98. 230th ACS meeting, Washington DC, Aug. 28-Sept. 1, 2005, "Finite Size Scaling for Critical Phenomena in Negative Ion Clusters"
99. Casper College-Texas A M University Quantum Optics Summer Workshop, August 14-August 20, 2005, "Finite Size Scaling in Quantum Mechanics"
100. 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"
101. Stanford University, CA, Department of Chemistry, June, 23, 2005, "Finite Size Scaling in Quantum Mechanics"
102. Purdue University, Computer Science and Engineering Spring 2005 Seminar Series, April 27, 2005 "Quantum Computing"



103. Department of Chemistry, Purdue University, West Lafayette "Finite Size Scaling in Quantum Mechanics", March 9, 2005.
104. 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"
105. Department of Chemistry, Technion Haifa 32000, Israel, July 27, 2004 "Tuning the Entanglement for magnetic Systems"
106. Department of Chemistry, Technion Haifa 32000, Israel, July 25, 2004 "Finite Size Scaling and Stability of Atomic and Molecular Ions"
107. Department of Chemistry, Purdue University, West Lafayette "Finite Size Scaling in Quantum Mechanics", March 24, 2004.
108. Kansas State University, Department of Chemistry Manhattan KS 66506-3701,"Finite Size Scaling for Stability of Atomic and Molecular Systems", March 18, 2004
109. WISICT 2004, Winter International Symposium on Information and Communication Technologies, Cancun, Mexico, January 5th-8th, 2004"Scaling of Entanglement at Quantum Phase Transitions"
110. WISICT 2004, Winter International Symposium on Information and Communication Technologies, Cancun, Mexico, January 5th-8th, 2004Chair: Workshop on Quantum Information Processing
111. Department of Mathematics, Purdue University, West Lafayette "Finite Size Scaling in Quantum Mechanics", October 3, 2003.
112. NASA JET PROPULSION LABORATORY, California Institute of Technology,"Scaling of Entanglement at Quantum Phase Transitions", August 15, 2003.
113. Workshop on Quantum Computing, "Tuning the Entanglement for magnetic Systems", University of Notre Dame, Notre Dame, IN, August 7, 2003
114. 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"
115. 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)
116. Florida State University, Department of Chemistry, "Quantum Critical Phenomena and Stability of Atomic and Molecular Ions"(invited by Prof. Sanford Safron)
117. The University of British Columbia, Department of Chemistry, Vancouver, Canada, June 10, 2002"Finite Size Scaling and Renormalization Group for Quantum Critical Phenomena"
118. 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"
119. 2002 DAMOP Annual Meeting, May 29-June 1 Williamsburg, VA meeting of the "Finite Size Scaling for Atomic and Molecular Systems"

120. University of Wisconsin-Madison, Department of Chemistry, Madison, WI, May 20, 2002, "Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
121. ONR Program Review, Arlington, Virginia, April 30- May 3, 2002 "Critical Phenomena and Renormalization Group Approach for Electronic Structure calculations"
122. Yale University, Department of Physics, New Haven, CT, April 22, 2002 "Finite Size Scaling for Quantum Critical Phenomena"
123. Carnegie Mellon University, Department of Chemistry, Pittsburgh, Pennsylvania, April 11, 2002. "Quantum phase transitions and Stability of atomic and molecular systems"
124. APS March Meeting 2002, Indianapolis, IN, March 18, 2002 Session A31 (Chemical Physics of Complex Systems) "Finite Size Scaling in Quantum Mechanics"
125. APS March Meeting 2002, Indianapolis, IN, March 20, 2002 Session M20 (One Dimensional Theory) "Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
126. Sanibel Symposium 2002 in Quantum Chemistry, Florida, February 23, 2002, Chair of plenary session on Multi-Scale Simulation.
127. Illinois Institute of Technology, Department of Biological, Chemical and Physical Sciences, Chicago, IL, February 20, 2002 "Finite Size Scaling for Quantum Critical Phenomena"
128. Purdue University, CS& E Spring 2002 Seminar Series, February 13, 2002 "Finite Size Scaling for Quantum Critical Phenomena"
129. Department of Chemistry, University of Michigan, Ann Arbor, MI, November 8, 2001 "Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
130. Department of Chemistry, Wayne State University, Detroit, MI, November 7, 2001 "Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
131. Department of Chemistry, Rutgers University, Piscataway, NJ, June 19, 2001 "Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
132. Sanibel Symposium 2001 in Quantum Chemistry Florida, February 28, 2001 "Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
133. Purdue University, Department of Chemistry West Lafayette, IN, January 17, 2000 "Quantum Phase Transitions and Stability of Atomic and Molecular Ions".
134. Department of Chemistry, Hebrew University, Jerusalem Israel, November 28, 2000 "Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
135. Department of Chemistry, Ben Guroun University, Israel November 15, 2000 "Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
136. Advances in Finite Time Thermodynamics, Jerusalem, Israel November 12-14, 2000 "Quantum Phase Transitions at  $T=0$ ".

137. 2000 Midwest Thermodynamics and Statistical Mechanics Conference, Minneapolis, Minnesota, May 14-16, 2000."Finite Size Scaling for Critical Parameter of Simple Diatomic Molecules"
138. Department of Chemistry, Wabash College, Crawfordsville, IN 47933, Tuesday Feb. 29, 2000 "Recent Advances in Electronic Structure Theory".
139. Department of Chemistry, Indiana University Bloomington, Indiana 47405, Thursday, September 23, 1999"Phase Transitions and Stability of Atomic and Molecular Ions."
140. Department of Chemistry and Physics, Indiana University, Bloomington, Indiana 47405, Friday, September 24, 1999"Finite Size Scaling in Quantum Mechanics".
141. Technion, Department of Chemistry Haifa 32000, Israel, Sunday June 13, 1999 "Recent Advances in Density Functional Theory".
142. The Ohio State University Department of Chemistry Columbus, OH 43210, Monday, April 26, 1999"Phase Transitions and Stability of Atomic and Molecular Ions".
143. Purdue University, Department of Physics, West Lafayette, IN, January 29, 1999 "Phase Transitions and Stability of Atomic and Molecular Ions".
144. University of Illinois at Urbana-Champaign, Department of Chemistry Urbana, IL, December 2, 1998"Phase Transitions and the Stability of Atomic and Molecular Ions".
145. Purdue University, Department of Chemistry West Lafayette, IN, September 7, 1998 "Phase Transitions and Stability of Atoms and Molecules".
146. 31st Midwest Theoretical Chemistry Conference Department of Chemistry, Purdue University Chair of the Conference.
147. University of California UCLA, Department of Chemistry Los Angeles, CA, March 11, 1998 "Phase Transitions and Stability of Atoms and Molecules".
148. The American Physical Society - 1998 March Meeting, Los Angeles, CA 16-20 March, 1998" Phase Transitions and Stability of Atomic and Molecular Negative Ions".
149. Southern Methodist University Department of Chemistry Dallas, Texas, April 23, 1998" Phase Transitions and Stability of Atoms and Molecules".
150. Hebrew University, Department of Chemistry Jerusalem, Israel, December 22, 1997 "Phase Transitions and Stability of Atoms and Molecules".
151. Technion, Department of Chemistry Haifa, Israel, December 23, 1997 "Phase Transitions and Stability of Atoms and Molecules".
152. Ninth Annual Conference on Recent Developments in Electronic Structure Methods Cornell University, Ithaca, NY, May 31-June 2, 1997 "Finite Size Basis Set Scaling Ansatz for Atoms".
153. 30th Midwest Theoretical Chemistry Conference University of Illinois, Urbana-Champaign, May 22-24, 1997 "Comparison of Pivot Methods for Global Optimization
154. The American Physical Society - 1997 March Meeting Kansas City, MO 17-21 March, 1997 "A New Approach for Global Optimization".
155. 29th Midwest Theoretical Chemistry Conference Indiana University-Purdue University Indianapolis, May 30- June 1, 1996" A New Approach to Global Minimization".

156. The American Physical Society: Atomic, Molecular and Optical Physics Indianapolis, Indiana, April 2, 1996 "Critical Phenomena for Electronic Structure at the Large-D limit".
157. The University of Illinois at Chicago Department of Chemistry Chicago, Illinois, March 7, 1996 "Dimensional Renormalization for the Treatment of Electron Correlation".
158. Purdue University: The Dean's Freshman Honors Seminar (SCI 110), Nov. 20, 1995 "New Challenges in Quantum Chemistry".
159. 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".
160. Technion, Physics Department Haifa, Israel, June 13, 1995 "Dimensional Renormalization for Electronic Structure of Atoms and Molecules".
161. Regensburg University, Institute for Theoretical Chemistry Regensburg, Germany, May 22, 1995 "Dimensional Renormalization for Electronic Structure of Atoms and Molecules".
162. NATO Advanced Research Workshop on New Methods in Quantum Theory Halkidiki, Greece, May 14-19, 1995 "Dimensional Renormalization for Electronic Structure Calculations".
163. Northwestern University, XXVIII Midwest Theoretical Chemistry Conference Evanston, Illinois, May 11-13, 1995 "Charge Renormalization at the Large-D Limit for Electronic Structure Calculations".
164. Purdue University, Department of Physics West Lafayette, IN March 20, 1995 "Molecules and Clusters".
165. Oregon State University, Department of Chemistry Corvallis, Oregon, April 14, 1993 "Electronic Structure Calculations by Density Functional Theory and Dimensional Scaling Methods".
166. Harvard University, Dudley Herschbach's 60th Birthday Cambridge, MA, July 1992 "Dimensional Scaling the Quasi stationary States".
167. Cambridge University, Department of Chemistry Cambridge, England, June 1992 "Electronic Structure Calculations by Density Functional and Dimensional Scaling".
168. Cornell University, Department of Physics Ithaca, NY, March 3, 1992 "Electronic Structure Calculations by Density Functional and Dimensional Scaling".
169. M.I.T., Department of Chemistry Cambridge, MA, October 30, 1991 "Tunneling in Multi-Dimensional Systems".
170. New York University, Department of Physics New York, New York, October 21, 1991 "Dimensional Scaling Method in Atomic and Molecular Physics".
171. Orsted Institute, Department of Chemistry Copenhagen, Denmark, June 1991 "Conference in Dimensional Scaling in Chemical Physics "Symmetry Breaking and Electronic Exchange Energy".

### **Other Presented Papers**

- 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 (QuICS). 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 Hefeng 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, Córdoba, 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 (H<sub>2</sub>O)<sub>N</sub> 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, 1998 Talk: 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, 1998 Poster: 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 Ansatz for Atoms.
- Ninth Annual Conference on Recent Developments in Electronic Structure Methods Cornell University, Ithaca, NY, May 31-June 2, 1997 Poster: Finite Size Basis Set Scaling Ansatz for Atoms.
- 30th Midwest Theoretical Chemistry Conference University of Illinois, Urbana-Champaign, May 22-24, 1997 Poster: 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, 1996 Poster: 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.