

Curriculum Vita

Sabre Kais

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EDUCATION AND PROFESSIONAL EXPERIENCE

- 2014-Present External Research Professor at Santa Fe Institute
2002-Present Full Professor of Chemical Physics, Purdue
2010-Present Courtesy Appointment as Professor of Physics, Purdue
2005-Present Courtesy Appointment as Professor of Computer Sciences, Purdue
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 80th 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

- 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-present (Quantum Annealing)
- Yuchen Wang (Physics) 2017-Present (Quantum Entanglement)
- Rongxin Xia (Physics) 2016-Present (Quantum Computing)
- Teng Bian (Physics) 2016-Present (Quantum Information)
- Kenneth Miller (Computer Science) 2017-Present (Quantum Algorithms)
- 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 Vandrevalla (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. Jiaxiang 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-present (Finite Size Scaling)
- Dr. Jiang Wang, August 2015-present (Professor Hefei, Quantum Computing)
- Dr. Nan Jiang, August 2015-present (Professor Hefei, Quantum Entanglement and Computing)
- Dr. Merid Legesse Belayneh, 2015-Present (Quantum Materials for Solar Energy)
- Dr. Zixuan Hu, 2016-Present (Quantum Coherence and Computing)
- Dr. Shuhao Yeh, 2016-Present (Quantum Coherence for Quantum Devices)
- Dr. Kumar Ghosh, 2018-Present (Quantum Machine Learning)
- Dr. Vivek Dixit, 2019-present (Quantum Machine Learning)
- Dr. Yijue Ding 2018-Present (Quantum Entanglement)

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 Pothen and Ashraf Alam (Co-PIs)
- 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)
- 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).
- Soar Technology, Inc., "Resisting Adversarial Attacks with Quantum Machine Learning", \$45,000 04/01/2019 - 09/30/2019, Sabre Kais (PI).

RESEARCH PROGRAM

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

- **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.

- Near Term Applications of Quantum Machine Learning Techniques to Many-body Systems:** Quantum machine learning – a hybridization of classical machine learning techniques with quantum computation – is emerging as a powerful approach that may have impactful applications in chemistry and Physics. This program will leverage our group's demonstrated expertise in quantum computation, machine learning and quantum theory to tackle important and challenging problems in quantum chemistry and Physics with quantum machine learning tools. We focus on three major development ideas for quantum machine learning algorithms, with applications in various problems in quantum chemistry and physics: 1. A hybrid quantum algorithm employing a restricted Boltzmann machine to obtain accurate molecular potential energy surfaces. 2. A way to realize non-linear activation functions in a quantum neural network model applied to finding the ground state energy for many-body systems. 3. A quantum machine learning algorithm to classify quantum states based on entanglement.

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 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, 3990-3998 (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. 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. Germann, and D.R. Herschbach, Large-Dimension Limit Yields Generic Potential Curves for H_2^+ , H_2 , HHe^+ , and He_2^{++} , 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, 491-294 (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 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).
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 Fe(CH₂O)⁺ and Fe(CH₂S)⁺ 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).
 48. M. El-Batanouny, G. Murthy, C.R. Willis, S. Kais and V. Staemmler, "Feasibility of Measuring Surface Electron Spin Dynamics by Inelastic Scattering of Metastable Helium Atoms, Phys. Rev. B 58, 7391-7402 (1998).
 49. P. Serra, J.P. Neirotti and S. Kais, "Electronic Structure Critical Parameters For the Lithium Isoelectronic Series", Phys. Rev. Letters 80, 5293-5296 (1998).
 50. Shi QC, Zhang SM, Cho H, Kezun X, Jia-Ming L and Kais S, "Relativistic structure description and relaxation effect on krypton $4p(5)(P-2(3/2,1/2))5s$ excitation at small squared momentum transfer", J Phys. B. 31, 4123 (1998).
 51. P. Serra, J.P. Neirotti and S. Kais, "Finite Size Scaling in Quantum Mechanics", J. Phys. Chem. A 102, 9518-9522 (1998).
 52. Sabre Kais, Juan Pablo and Pablo Serra, "Phase transitions and the stability of atomic and molecular ions", International Journal of Mass Spectrometry 182/183, 23-29 (1999).
 53. Pablo Nigra and Sabre Kais, "Pivot methods for global optimization: A study of water clusters H_2N with $2 < N < 33$ ", Chem. Phys. Letters, 305, 433-438 (1999).
 54. A.V. Sergeev and S. Kais, "Variational Principle for Critical Parameters of Quantum Systems", J. Phys. A. 32, 6891-6896 (1999).
 55. Alexei Sergeev and Sabre Kais, "Critical nuclear charges for N-electron atoms", Int. J. Quant. Chem. 75,533-542 (1999).
 56. Sabre Kais and Pablo Serra, "Quantum Critical Phenomena and Stability of Atomic and Molecular Ions", Int. Rev. Phys. Chem. Vol 19, 97-121 (2000).
 57. Pablo Serra and Sabre Kais, "Data collapse for the Schrodinger equation", Chem. Phys. Letters, 319, 273-277 (2000).
 58. Pablo Serra, Sabre Kais and Juan P. Neirotti, "Finite size scaling method for the stability of atomic and molecular ions", PHYSICA A 283, 65-73 (2000).
 59. Qicun Shi and Sabre Kais, "Finite size scaling for critical parameters of simple diatomic molecules", Mol. Phys. 98, 1485-1495 (2000).
 60. Imad Ladadwa and Sabre Kais, "Critical Behavior of Electron Impact Ionization of Atoms", Int. J. Quantum Chem. 80, 575-581 (2000).
 61. Sabre Kais and Qicun Shi, "Quantum Criticality and Stability of Three-Body Coulomb Systems", Phys. Rev. A (Rapid Communications) 62, 060502-5 (2000).
 62. Ricardo Sauerwein and Sabre Kais, "Quantum Critical Phenomena in the Schrodinger Formulation: Mapping to Classical Lattices", Chem. Phys. letters 333, 451-458 (2001).
 63. A.V. Sergeev and S. Kais, "Resonance States of Atomic Anions", Int. J. Quantum Chemistry, 82, 255-261 (2001).

64. Q. Shi, S. Kais, F. Remacle and R.D. Levine, "On the Crossing of Electronic Energy Levels of diatomic Molecules at the Large-D Limit", *J. Chem. Phys.* 114, 9697-9705 (2001).
65. Q. Shi, S. Kais, F. Remacle and R.D. Levine, "Electronic Isomerism: Symmetry Breaking and Electronic Phase Diagrams for Diatomic Molecules at the Large-Dimension Limit ", *CHEMPHYSICHEM* 2, 434-442 (2001).
66. Q. Shi and S. Kais, " Quantum Criticality at the Large Dimensional Limit: Three-Body Coulomb Systems", *Int. J. Quantum Chem.* 85, 307-314 (2001).
67. Pablo Nigra, Marcelo Carignano and Sabre Kais," Study of phase changes in water octamer using the parallel tempering and multihistogram methods", *J. Chem. Phys.* 115, 2621-2628 (2001).
68. Pablo Serra, Sabre Kais and Nimrod Moiseyev," Crossover phenomena and resonances in quantum systems", *Phys. Rev. A* 64, 0262502-1-6 (2001).
69. Ricardo A. Sauerwein and Sabre Kais," Quantum criticality for few-body systems: Path integral approach ", *Phys. Rev. E* 64, 056120-1-6 (2001).
70. Stephen D. Belair, Sabre Kais, and Joseph S. Francisco," Potential Energy Surface for the Hydroperoxy and Water Radical Complex", *Molecular Physics* 100, 247-253 (2002).
71. Qicun Shi and Sabre Kais," Lifetimes of Metastable Spherical Carbon Cluster Dianions", *Molecular Physics* 100, 475-481 (2002).
72. J. X. Wang, Sabre Kais and R.D. Levine," Real-space renormalization group study of the Hubbard model on a non-bipartite lattice", *International Journal of Molecular Sciences* 3, 4-16 (2002).
73. S. Kais, "Finite Size Scaling in Quantum Mechanics", *Proceedings of the 2002 International Conference on Computational Nanoscience and Nanotechnology, ICCN 2002* p. 474-477 (2002).
74. Qicun Shi and Sabre Kais,"The repulsive Coulomb barrier along a dissociation path of the BeC_4^{2-} dianion", *J. Am. Chem. Soc.* 124, 11723-11729 (2002).
75. J. X. Wang, Sabre Kais, F. Remacle and R.D. Levine,"Size effects in the electronic properties of finite arrays of exchange coupled quantum dots", *J. Phys. Chem. B. (Letters)* 106, 12847-12850 (2002).
76. J.X. Wang and Sabre Kais, "Finite Size Scaling for Mott metal-insulator transition on half-filled non-partite lattice", *Phys. Rev. Rapid Communications*, B66, 081101-1 (2002)
77. S. Kais, "Finite Size Scaling in Quantum Mechanics", *Proceedings of the 2002 International Conference on Computational Nanoscience and Nanotechnology, ICCN 474-477* (2002).
78. S. Kais and P. Serra, "Finite Size Scaling for Atomic and Molecular Systems", *Adv. Chem. Phys. Volume* 125, 1-100 (2003).
79. J. X. Wang and Sabre Kais, "Metal-insulator transition in Hubbard model on a triangular lattice with disorders: Renormalization group approach", *Int. J. Quantum Chem.* 93, 360-374 (2003).
80. Pablo Serra and Sabre Kais, "Finite Size Scaling for Critical Conditions for Stable Dipole-Bound Anions" *Chemical Physics Letters* 372, 205-209 (2003).

81. Omar Osenda, Zhen Huang and Sabre Kais, "Tuning the Entanglement for a 1D Magnetic System with Anisotropic Coupling and Impurities" , Phys. Rev. A 67, 062321-4 (2003).
82. J. X. Wang and S. Kais "Combined effects of disorders and electron-electron interactions upon metal-insulator transition in 2D non-bipartite lattice", Physics Letters A 316, 265-270 (2003).
83. Qicun Shi, Stephen D. Belair, Sabre Kais, and Joseph S. Francisco, "On the Interaction between Atmospheric radicals and Cloud Droplets: A Molecular Picture of the Interface, PNAS 100, 9686-9690 (2003).
84. Jiaxiang Wang and Sabre Kais, "Scaling of entanglement in finite arrays of exchange-coupled quantum dots", Int. J. Quant. Information Vol 1 (3), 375-387 (2003).
85. Qicun Shi, Sabre Kais and Dudley R. Herschbach, "Electron localization-delocalization transitions in dissociation of the C4 anion: A large-D analysis", J. Chem. Phys. 120, 2199-2207 (2004).
86. Zhen Huang, Omar Osenda and Sabre Kais, "Entanglement of formation for one-dimensional magnetic systems with defects", Physics Letters A 322, 137-145 (2004).
87. Sabre Kais and Pablo Serra, "Finite Size Scaling in Quantum Mechanics", in Progress in Quantum Physics Research. Edited by V. Krasnoholovets and F.H. Columbus, Nova Science Publishers, Chap 6, 155-164 (2004).
88. Alejandro Ferron, Pablo Serra and Sabre Kais, "Finite Size Scaling for Critical Conditions for Stable Quadrupole-Bound Anions , J. Chem. Phys. 120, 8412-8419 (2004).
89. Jiaxiang Wang and Sabre Kais, "Scaling of entanglement at quantum phase transition for two-dimensional array of quantum dots", Phys. Rev. A 70, 022301-1 022301-4 (2004).
90. Qicun Shi and Sabre Kais, "Finite Size Scaling for the Atomic Shannon-Information Entropy", J. Chem. Phys. 121, 5611-5617 (2004).
91. Qicun Shi and Sabre Kais, "Discontinuity of Shannon-Information Entropy for Two-Electron Atoms", Chem. Phys. 309, 127-131 (2005).
92. Zhen Huang and Sabre Kais, "Dynamics of Entanglement for One-Dimensional Spin Systems in an External Time-Dependent Magnetic Field", In. J. Quant. Information 3, 483-500 (2005).
93. Qicun Shi, Sabre Kais, and Joseph Francisco "Graph Theory for Fused Cubic Clusters of Water Dodecamer", J. Phys. Chem. A 109, 12036-12046 (2005).
94. Zhen Huang and Sabre Kais, "Entanglement as Measure of Electron-Electron Correlation in Quantum Chemistry Calculations", Chem. Phys. Letters 413, 1 (2005).
95. Zhen Huang and Sabre Kais, "Entanglement Evolution of One-dimensional Spin Systems in External Magnetic Fields", Phys, Rev. A 73, 022339 (2006).
96. Zhen Huang, Gehad Sadiek and Sabre Kais, "Time evolution of a single spin inhomogeneously coupled to an interacting spin environment", J. Chem. Phys. 124, 144513 (2006).

97. Hefeng Wang and Sabre Kais, "Entanglement and Quantum Phase Transition in a One-Dimensional System of quantum Dots with Disorder" *Int. J. Quantum Information* 4, 827-835 (2006).
98. Hefeng Wang and Sabre Kais, "Quantum Teleportation in One-Dimensional Quantum Dots System" *Chem. Phys. Letters* 421, 338 (2006).
99. Sabre Kais, Crraig Wenger and Qi Wei, "Quantum criticality at the infinite complete basis set limit: A thermodynamic analog of the Yang and Lee theorem" *Chem. Phys. Letters* 423, 45 (2006).
100. Qi Wei, Sabre Kais and Nimrod Moiseyev "New Stable Multiply Charged Negative Atomic Ions in Linearly Polarized Superintense Laser Fields" *Communication: J. Chem. Phys.* 124, 201108 (2006).
101. Zhen Huang, Hefeng Wang and Sabre Kais, "Entanglement and Electron Correlation in Quantum Chemistry Calculations", *Journal of Modern Optics*, 53, 2543-2558 (2006).
102. Sabre Kaise, *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).
103. Uri Peskin, Zhen Huang and Sabre Kais, "Internal Entanglement Amplification by External Interactions", *Phys. rev. A* 76, 012102 (2007).
104. Hefeng Wang and Sabre Kais, "Quantum Entanglement and Electron Correlation in Molecular Systems", *Israel Journal of Chemistry*, 47, 59-65 (2007).
105. Qi Wei, Sabre Kais and Nimrod Moiseyev "Frequency-dependent stablization of He- by a superintense laser field" *Phys. Rev. A* 76, 013407 (2007).
106. Qi Wei, Sabre Kais and Dudley Herschbach, "Dimensional Scaling Treatment of Stability of Atomic and Anions Induced by Superintense Laser Fields" *J. Chem. Phys.* 127, 094301 (2007).
107. A. Ferron, P. Serra, and S. Kais, "Critical conditions for stable dipole-bound dianions", *J. Chem. Phys.* 128, 044307 (2008).
108. Winton Moy, Sabre Kais and Pablo Serra, "Finite Size Scaling with Gaussian Basis Sets", *Molecular Physics* 106, 203-212 (2008).
109. Sabre Kais and Nicholas Handy, A special issue in honour of Professor Raphael D. Levine – Preface *Mol. Phys.* 106, 191 (2008).
110. A. Ferron, P. Serra, and S. Kais, "Critical Conditions for Stability of Hydrogen-Antihydrogen Like Systesm", *Phys. Rev. A* 77, 052505 (2008).
111. W. Moy, M. Carignano and S. Kais, "Finite Size Scaling with the Finite Element Method", *J. Phys. Chem.* 112, 5448-5452 (2008).
112. H. Wang, S. Kais, Alan Aspuru-Guzik and Mark R. Hoffmann, "Quantum Algorithm for Obtaining the Energy Spectrum of Molecular Systems", *Physical Chemistry Chemical Physics*, 10, 5388-5393 (2008).
113. Omar Osenda, Pablo Serra and Sabre Kais, "Dynamics of Entanglement for Two-Electron Atoms", *Int. J. Quantum Information*, 6, 303-316 (2008).
114. A. Ferron, P. Serra, and S. Kais, "Dimensional scaling for stability of two particles in a dipole field", *Chem. Phys. Letters*, 461, 127-130 (2008).
115. Gehad Sadiekabc, Zhen Huang, Omar Aldossary and Sabre Kais, "Nuclear-induced time evolution of entanglement of two-electron spins in anisotropically couple quantum dot", *Mol. Phys.* 106, 1777-1786 (2008).

116. Qi Wei, Sabre Kais, and Dudley Herschbach, "Dimensional scaling treatment of stability of simple diatomic molecules induced by super-intense, high-frequency laser fields", *J. Chem. Phys.* 129, 214110-8 (2008).
117. Sangchul Oh, Zhen Huang, Uri Peskin and Sabre Kais, "Entanglement, Berry phases, and level crossings for the atomic Breit-Rabi Hamiltonian ", *Phys. Rev. A* {bf 78}, 062106-7 (2008).
118. Zhen Huang, Jing Zhu and Sabre Kais, "Simulated Quantum Computation of Global Minima", *Molecular Physics* 107, 2015 (2009).
119. S.Y. Du, J.S. Francisco, S. Kais, ``Study of electronic structure and dynamics of interacting free radicals influenced by water", *J. Chem. Phys.* 130, 124312 (2009).
120. H. Wang and S. Kais, ``Quantum Teleportation in Quantum Dots System", *Handbook of Nanophysics*. Edited by Klaus Sattler (2009).
121. M. Carignano, A. Mahammad and S. Kais, ``Temperature Dependent Electron Binding in H₂O₈, *J. Phys. Chem. A* 113, 10886 (2009).
122. E. Antillon, W. Moy, Q. Wei and S. Kais, ``Comparison Study of Finite Element and Basis Set Methods for Finite Size Scaling", *J. Chem. Phys.* 131}, 104105 (2009).
123. Qing Xu, Sabre Kais, maxim Naumov and Ahmed Sameh, ``Exact calculation of entanglement in a 19-site two-dimensional spin system", *Phys. Rev. A.* 81, 022324 (2010).
124. S. Kais, Q. Wei, and Y. Chen, ``Entanglement Switch in an Optical Lattice", *J. Chem. Phys.* 132, 121104 (2010).
125. Sabre Kais, ``Finite Size Scaling for Criticality of the Schrodinger Equation", ``Solving the Schrodinger $\frac{1}{2}$ dinger equation: has everything been tried", Edited by Paul Popelier (*Imperial College Press, London, 2011*).
126. Jing Zhu, Sabre Kais, Patrick Rebentrost and Alan Aspuru-Guzik, ``Modified-scaled hierarchical equation of motion approach for the study of quantum coherence in photosynthetic complexes", *J. Phys. Chem. B* 115, 1531 (2011).
127. Anmer Daskin and Sabre Kais, ``Group Leaders Optimization", *Mol. Phys.* 109, 761 (2011).
128. Anmer Daskin and Sabre Kais, ``Decomposition of unitary matrices for finding quantum circuits", *J. Chem. Phys.* 134, 144112 (2011).
129. Mikhail Lemeshko, Mustafa Mustafa, Sabre Kais and Bretislav Friedrich, "Supersymmetric factorization yields exact solutions to the molecular Stark-effect problem for stretched states", *Phys. Rev. A* 83, 043415 (2011).
130. Qi Wei, Sabre Kais, Bretislav Friedrich and Dudley Herschbach, "Entanglement of polar molecules in pendular states", *J. Chem. Phys.* 134, 124107 (2011).
131. X. Qing, G. Sadiq and S. Kais, "Dynamics of entanglement in a two-dimensional spin system", *Phys. Rev. A* 83, 062312, (2011).
132. Mikhail Lemeshko, Mustafa Mustafa, Sabre Kais and Bretislav Friedrich, "Supersymmetry identifies molecular Stark states whose eigenproperties can be obtained analytically", *New Journal of Physics* 13, 063036 (2011).
133. Alkurtass Bedoor; Sadiq Gehad; Kais Sabre, "Entanglement dynamics of one-dimensional driven spin systems in time-varying magnetic fields ", *Physical Reveiw A* , 84, 022314 (2011).

134. Shu-Hao Yeh; Jing Zhu, and Sabre Kais, Population and coherence dynamics in light harvesting complex II (LH2), *J. Chem. Phys.* 137, 084110 (2012).
135. Jing Zhu, Sabre Kais, Alan Aspuru-Guzik, Sam Rodrigues, Ben Brock, and Peter Love, Multipartite quantum entanglement evolution in photosynthetic complexes, *J. Chem. Phys.* 137, 074112 (2012).
136. Gehad Sadiq, Qing Xu; and Sabre Kais, Tuning entanglement and ergodicity in two-dimensional spin systems using impurities and anisotropy, *Phys. Rev. A* 85, 042313 (2012).
137. Ross Hoehn, Jiayang Wang; and Sabre Kais, Dimensional scaling treatment with relativistic corrections for stable multiply charged atomic ions in high-frequency super-intense laser fields *J. Chem. Phys.* 136, 034114 (2012).
138. Yudong Cao, Anmer Daskin, Steven Frankel Kais, and Sabre Kais, Quantum circuit design for solving linear systems of equations, *Mol. Phys.* 110, 1675 (2012).
139. Anmer Daskin; Ananth Grama; Giorgos Kollias and Sabre Kais, Universal programmable quantum circuit schemes to emulate an operator. *Journal of chemical physics*, 137, 234112 (2012).
140. Pablo Serra, and Sabre Kais, Ground-state stability and criticality of two-electron atoms with screened Coulomb potentials using the B-splines *J. Phys. B* 45, 235003 (2012).
141. Bretislav Friedrich, Sabre Kais, David Mazziotti, Scaling Mount Impossible: A Festschrift for Dudley Herschbach PREFACE, *Molecular Physics*, 110, 1537 (2012).
142. Jing Zhu, Sabre Kais, Qi Wei, Dudley Herschbach, Bretislav Friedrich, Implementation of Quantum Logic Gates Using Polar Molecules in Pendular States, *J. Chem. Phys.* 138, 024104 (2013)
143. Yudong Cao, Anargyros Papageorgiou, Iasonas Petras, Joseph Traub, Sabre Kais, Quantum algorithm and circuit design solving the Poisson equation, *New J. Phys.* 15, 013021 (2013).
144. Fahhad Alharbi and Sabre Kais, Quantum criticality analysis by finite-size scaling and exponential basis sets, *Phys. Rev. E* 87, 043308 (2013).
145. Mikhail Lemeshko, Roman V. Krems, John M. Doyle, Sabre Kais, Manipulation of Molecules with Electromagnetic Fields, *Mol. Phys.* 111, 1648 (2013).
146. Mauro Faccin, Tomi Johnson, Jacob Biamonte, Sabre Kais, Piotr Migda,, Degree Distribution in Quantum Walks on Complex Networks, *Phys. Rev. X*, 3, 041007 (2013).
147. Pablo Serra, Marcelo Carignano, Fahhad Alharbi, Sabre Kais, Quantum Confinement and Negative Heat Capacity, *Europhysics letters*, 104, 16004 (2013).
148. Edwin Antillon, Birgit Wehefritz-Kaufmann, Sabre Kais, Avalanches in the Raise and Peel model in the presence of a wall, *J. Phys. A: Math. Theor.* 46, 265001 (2013).
149. Ankang Li, Jiayang Wang, Na Ren, Pingxiao Wang, Wenjun Zhu, Xiaoya Li, RossHoehn, Sabre Kais , Harmonic generation from free electrons in intense laser fields: classical versus semi-classical theory, *Laser Phys.* 24, 015302 (2013).

150. Ankang Li, Jiaxiang Wang, Na Ren, Pingxiao Wang, Wenjun Zhu, Xiaoya Li, Ross Hoehn, Sabre Kais, The interference effect of laser-assisted bremsstrahlung emission in Coulomb fields of two nuclei, *Journal of Applied Physics*, 114, 124904 (2013).
151. James Pauls, Yiteng Zhang, Gennady Berman, Sabre Kais, Quantum coherence and entanglement in the avian compass, *Physical Review E*, 87, 062704 (2013).
152. Anmer Daskin, Ananth Grama, Sabre Kais, A universal quantum circuit scheme for finding complex eigenvalues, *Quantum Information Processing* 1, 21 (2013).
153. Gehad Sadiq and Sabre Kais, Persistence of entanglement in thermal states of spin systems, *J. Phys. B*, 46, 245501 (2013).
154. Ross Hoehn and Sabre Kais, Using Quantum Games To Teach Quantum Mechanics, Part 1, *J. Chem. Education* 91, 417 (2014).
155. Ross Hoehn and Sabre Kais, Using Quantum Games To Teach Quantum Mechanics, Part 2, *J. Chem. Education* 91, 423 (2014).
156. Yiteng Zhang, Gennady Berman and Sabre Kais, Sensitivity and entanglement in the avian chemical compass, *Physical Review E*, 90, 042707 (2014).
157. Rishabh Chandra, N. Tobias Jacobson, Jonathan E. Moussa, Steven H. Frankel, Sabre Kais, Quadratic constrained mixed discrete optimization with an adiabatic quantum optimizer, *Phys. Rev. A* 90, 012308 (2014).
158. Vladimir U. Nazarov, Fahhad Alharbi, Timothy Fisher, and Sabre Kais, Coupled plasmon - phonon excitations in extrinsic monolayer graphene, *Phys. Rev. B*. 89, 195423 (2014).
159. A K Li, J X Wan¹, N Ren, W J Zhu, X Y Li², Ross Hoehn, and Sabre Kais, Harmonic generation from free electrons in intense laser fields: classical versus semi-classical theory, *Laser Phys.* 24, 015302 (2014).
160. A. Daskin, A. Grama, and S. Kais, A universal quantum circuit scheme for finding complex eigenvalues *Quantum Information Processing* 13, 333 (2014).
161. Jian Pan, Yudong Cao, Xiwei Yao, Zhaokai Li, Chenyong Ju, Hongwei Chen, Xinhua Peng, Sabre Kais, and Jiangfeng Du, Experimental realization of quantum algorithm for solving linear systems of equations, *Phys. Rev. A*. 89, 022313 (2014).
162. Ma Yong-Jun, Wang Jia-Xiang, Xu Xin-Ye, Wei Qi, and Sabre Kais, Error Analysis of the Density-Matrix Renormalization Group Algorithm for a Chain of Harmonic Oscillators, *Chines Phys. Lett.* 31, 060501 (2014).
163. F. Herrera, Y. Cao, Yudong, S. Kais and B. Whaley, Infrared-dressed entanglement of cold open-shell polar molecules for universal matchgate quantum computing, *New J. Phys.* 16, 075001 (2014).
164. Yongjun Ma, Jiaxiang Wang, Xinye Xu, Qi Wei, Wenjun Zhu, and Sabre Kais, A Density-Matrix Renormalization Group Study of a One-Dimensional Incommensurate Quantum Frenkel-Kontorova Model, *Journal of the Physical Society of Japan* 83, 094605 (2014).
165. Hoehn, Ross. D.; Schreder, Ashley. M.; Al Rez, Mohammed Fayez, An Agent-based Model Approach to Multi-phase Life-cycle for Contact Inhibited, Anchorage Dependent Cells, *Interdisciplinary Sciences-Computational Life Sciences*, 6, 312-322 (2014).

166. Dong Wang, Liu Ye, Sabre Kais, Multiparty-controlled remote preparation of four qubit cluster-type entangled states, EPL (submitted, 2014).
167. Yiteng Zhang, Sangchul Oh, Fahhad H. Alharbi, Greg Engel, Sabre Kais, Delocalized Quantum States Enhance Photocell Efficiency, Physical Chemistry Chemical Physics: PCCP, 17, 5743-5750 (2015).
168. Sangchul Oh, Sabre Kais, Transitionless driving on adiabatic search algorithm, J. Chem. Phys. 141, 224108 (2014).
169. Shu-Hao Yeh, Sabre Kais, Simulated two-dimensional electronic spectroscopy of the eight-bacteriochlorophyll FMO complex, J. Chem. Phys. 141, 234105 (2014).
170. Y. Cao, R. Babbush, J. Biamonte and S. Kais, Hamiltonian gadgets with reduced resource requirements, Phys. Rev. A 91, 2315 (2015).
171. Y. Zhang, S. Oh, F. Alharbi, G. Engel and S. Kais, Delocalized quantum states enhance photocell efficiency, Physical chemistry chemical physics, 17, 5743 (2015).
172. K.L. Brown, A. Daskin, S. Kais and J.P. Dowling, Reducing the number of ancilla qubits and the gate count required for creating large controlled operations, Quantum Information Processing, 14, 891 (2015).
173. 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).
174. Ross D. Hoehn, David Nichols, Hartmut Neven, and Sabre Kais, Neuroreceptor Activation by Vibration-Assisted Tunneling, Scientific Reports 5, 9990 doi:10.1038/srep09990 (2015).
175. Yiteng Zhang, Gennady Berman and Sabre Kais, The Radical Pair Mechanism and the Avian Chemical Compass, International Journal of Quantum Chemistry, 115, 15 (2015).
176. Carlo Motta, Fedwa El Mellouhi, Sabre Kais, Nouar Tabet, Fahhad Alharbi, Stefano Sanvito, Revealing the role of organic cations in hybrid halide perovskites CH₃NH₃PbI₃, Nature Communications, 6:7026 (2015).
177. Yiteng Zhang, Sangchul Oh, Fahhad H. Alharbi, Gregory S. Engel and Sabre Kais, Delocalized quantum states enhance photocell efficiency, Phys. Chem. Chem. Phys. 17, 5743 (2015).
178. Dong Wang, Ross D. Hoehn, Liu Ye and Sabre Kais, "Generalized Remote Preparation of Arbitrary m-qubit Entangled States via Genuine Entanglements", Entropy 17, 1755-1774 (2015).
179. Sergey N. Rashkeev, Fedwa El-Mellouhi, Sabre Kais and Fahhad H. Alharbi, "Domain Walls Conductivity in Hybrid Organometallic Perovskites and Their Essential Role in CH₃NH₃PbI₃ Solar Cell High Performance", Scientific Reports, 5, 11467 (2015).
180. Fahhad H Alharbi, Sergey N Rashkeev, Fedwa El-Mellouhi, Hans P Luthi, Nouar Tabet, and Sabre Kais, An Efficient Descriptor Model for Designing Materials for Solar Cells, NPJ Computational Materials, 1, 15003 (2015)

181. G. R. Berdiyrov, M. El-Amine Madjet, F. El-Mellouhi, S. Kais, and F. M. Peeters, Effect of halide-mixing on the electronic transport in organometallic perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$, *Solar Energy Materials and Solar Cells* 148, 2 (2015).
182. Hans P. Luthi, Stefan Heinen, Gisbert Schneider, Andreas Glass, Martin P. Brandle, Rollin A. King, Edward Pyzer-Knapp, Fahhad H. Alharbi, and Sabre Kais, The Quantum Chemical Search for Novel Materials and the Issue of Data Processing: The InfoMol Project *Journal of Computational Science*, 418 (2015).
183. Kothand Rama, Kabalan, L., Abu-Omar, Mahdi, Kais, Sabre, Mechanism of Isomerization and Methyl Migration in Heterobimetallic RheniumIridium Complexes: Experimental and DFT Study, *American Chemical Society, Organometallics* 2016, 35, 605–611 (2016).
184. Mohamed El-Amine Madjet, Alexey V. Akimov, Fadwa El-Mellouhi, Golibjon R. Berdiyrov, Sahel Ashhab, Nouar Tabeta and Sabre Kais, Enhancing the Carrier Thermalization Time in Organometallic Perovskites by Halide Mixing, *Physical Chemistry Chemical Physics*, 18, 5219 (2016).
185. S. Oh, X. Hu, F. Nori and S. Kais, Singularity of the time-energy uncertainty in adiabatic perturbation and cycloids on Bloch sphere, *Scientific Reports* 6, 20824 (2016).
186. Raka Jovanovic, Sabre Kais, Fahhad H. Alharbi, Cuckoo Search Inspired Hybridization of the Nelder-Mead Simplex Algorithm Applied to Optimization of Photovoltaic Cells , *Appl. Math. Inf. Sci.* 10, No. 3, 961-973 (2016)
187. Mallikarjun Karra, Ketan Sharma, Bretislav Friedrich, Sabre Kais and Dudley Herschbach, Prospects for quantum computing with an array of ultracold polar paramagnetic molecules *J. Chem. Phys.* 144, 094301 (2016).
188. Ross Hoehn, Sachin Dilip Yeole, Sabre Kais, Joseph S. Francisco Analytic ab initio-based Molecular Interaction Potential for the $\text{BrO-H}_2\text{O}$ Complex *J. Chem. Phys.* 144, 204121 (2016).
189. Ross Hoehn, Marcelo Carignano, Sabre Kais, Chongjing Zhu, Jie Zhong, Xiao Cheng Zeng, Joseph S. Francisco, Ivan Gladich, Hydrogen Bonding and Orientation Effects on the Accommodation of Methylamine at the Air-Water Interface, *Journal of Chemical Physics*, 144, 214701 (2016).
190. Sergeev, Alexey, Jovanovic, Raka, Alharbi, Fahhad, H., Kais, Sabre, On the Divergence of Gradient Expansions for Kinetic Energy Functionals in the Potential Functional Theory, *Journal of Physics A: Mathematical & Theoretical*, 49, 285202 (2016).
191. Fedwa El-Mellouhi, El Tayeb Bentría, Sergey N Rashkeev, Sabre Kais and Fahhad H Alharbi, Enhancing Intrinsic Stability of Hybrid Perovskite Solar Cell by Strong, yet Balanced, Electronic Coupling, *Nature Materials*, Submitted (2016).
192. Fedwa El-Mellouhi, El Tayeb Bentría, Sergey N. Rashkeev, Sabre Kais and Fahhad H. Alharbi, Hydrogen Bonds: A New Mechanism for Tuning and Stabilizing Hybrid Organic and Inorganic Frameworks, *Nature Photonics*, Submitted (2016).
193. Wang, Dong, Hoehn, Ross, D., Ye, Liu, Kais, Sabre , Efficient Remote Preparation of Four-Qubit Cluster-Type Entangled State with Multi-Party Over

- Partially Entangled Channels, *International Journal of Theoretical Physics* 55, 3454-3466, 4 (2016).
194. Yudong Cao, Shuxian Jiang, Debbie Perouli and Sabre Kais , Solving Set Cover with Pairs Problem using quantum annealing, *Scientific Reports*: 6, 33957, (2016).
 195. Yudong Cao and Sabre Kais, Efficient estimation of perturbation error with cellular automaton, *New Journal of Physics*, submitted (2016).
 196. Wie, Qi, Cao, Yudong, Friedrich, Bretislav, Herschbach, Dudley and Kais, Sabre, Quantum Computation Using Arrays of N Polar Molecules in Pendular States, *ChemPhysChem*: 17, 1-10 (2016).
 197. El Mellouhi, Fedwa, Bentría, El Tayeb, Kais, Sabre; et al, Hydrogen Bonding: a Mechanism for Tuning Electronic and Optical Properties of Hybrid Organic-Inorganic Frameworks, *NPJ Computational Materials*: 2, 16035 (2016).
 198. Chongqin Zhu, Sabre Kais, Xiao Cheng Zheng, Joseph S. Francisco, and Ivan Gladich, Interfaces Select Specific Stereochemical Conformations: The Isomerization of Glyoxal at the Liquid Water Interface, *J. Am. Chem. Soc* Published Nov. 11 (2016).
 199. Yiteng Zhang, Aaron Wirthwein, Fahhad H. Alharbi, Gregory S. Engeld and Sabre Kais, Dark states enhance the photocell power via phononic dissipation, *Phys. Chem. Chem. Phys* 18, 31845 (2016).
 200. Rongxin Xia, Teng Bian, Sabre Kais, Electronic Structure Calculations and the Ising Machine, submitted *Nature Chemistry* (2016).
 201. El-Mellouhi, F.; Akande, A.; Kais, S.; et. al. Solar Cell Materials by Design: Hybrid Pyroxene Corner-Sharing VO₄ Tetrahedral Chains *Chemsuschem*; 10, 9, 1931-1942; DOI: 10.1002/cssc.201700121 (2017)
 202. Pichaandi, KR.; Kabalan, L.; Kais, S.; Abu-Omar, M., Ring flipping in Heterobimetallic Re-Ir Complexes and its Effect on Structural Isomerism: Dynamic NMR and DFT Study , *Journal of Organometallic Chemistry*; 843, 62-65; DOI: 10.1016/j.jorganchem.2017.05.030 (2017)
 203. Legesse, M.; El Mellouhi, F.; Kais, S.; et. al., Reduced Work Function of Graphene by Metal Adatoms, *Applied Surface Science*; 394, 98-107; DOI: 10.1016/j.apsusc.2016.10.097
 204. Wei, Q.; Wang, Px.; Kais, S: et. al., Pursuit of the Kramers-Henneberger Atom, *Chemical Physics Letters*; 683 240-246; DOI: 10.1016/j.cplett.2017.02.017 (2017)
 205. Pichaandi, KR.; Kabalan, L.; Kais, S.; et. al., Mechanism of Me-Re Bond Addition to Platinum(II) and Dioxygen Activation by the Resulting Pt-Re Bimetallic Center, *Inorganic Chemistry*; 56, 4,2145-2152; DOI: 10.1021/acs.inorgchem.6b02801 (2017)
 206. Alharbi, FH.; Kais, S., Kinetic Energy Density for Orbital-Free Density Functional Calculations by Axiomatic Approach, *International Journal of Quantum Chemistry*; 117, 12, DOI: 10.1002/qua.25373 (2017)
 207. Zhu, CQ; Zeng, XC; Kais, S; et.al., Interfaces Select Specific Stereochemical Conformations: The Isomerization of Glyoxal at the Liquid Water Interface, *Journal of the American Chemical Society*, 139; 1; DOI: 10.1021/jacs.6b10208 (2017)

208. Hoehn, R.D.; Nichols, D.E.; Kais, S. et.al., Experimental Evaluation of the Generalized Vibrational Theory of G Protein-Coupled Receptor Activation, *Proceedings of the National Academy of Sciences of the United States of America*; 114, 22 5595-5600; DOI: 202073/pnas.1618422114 (2017)
209. Wang, D.; Huang, A.J.; Hoehn, R.D.; Kais, S.; et.al, Entropic uncertainty relations for Markovian and non-Markovian processes under a structured bosonic reservoir, *Scientific Reports*; 7, 1066, DOI: 10.1038/s41598-017-01094-8 (2017)
210. Cao, Y.D.; Kais, S., Efficient Optimization of Perturbative Gadgets, *Quantum Information & Computation*; 17, 9-10, 779-809 (2017)
211. Daskin, Ammar; Kais, Sabre, An Ancilla-Based Quantum Simulation Framework for Non-Unitary Matrices, *Quantum Information Processing*: 16:1 DOI: 10.1007/s11128-016-1452-3 (2017)
212. Madjet, M. E.; Berdiyrov, G. R.; Kais, S.; et. al., Cation Effect on Hot Carrier Cooling in Halide Perovskite Materials, *J. Phys. Chem. Lett.*, 2017, 8 (18), 4439–4445 DOI:10.1021/acs.jpcclett.7b01732
213. Rolczynski, B.; Zheng, H.; Kais, S, et. al., Correlated Protein Environments Drive Quantum Coherence Lifetimes in Photosynthetic Pigment-Protein Complexes, *Chem* 4, 139-149, doi.org/10.1016/j.chempr.2017.12.009 (2018).
214. R. Xia, T. Bian and S. Kais, Electronic Structure Calculations and the Ising Hamiltonian, *The J. Phys. Chem. B*, 122, 3384-3395 (2018).
215. Zhong, Jie; Carignano, Marcelo; Kais, Sabre; Zeng, Xiao Cheng; Francisco, Joseph; Gladich, Ivan J., Tuning the Stereo and Solvation Selectivity at Interfacial and Bulk Environments by Changing Solvent Polarity: the Isomerization of Glyoxal in Different Solvent Environments, *Am. Chem. Soc.* 140, 5535-5543, (2018).
216. Hu,Z; Engel, G.S.; Kais, S., Connecting Bright and Dark States Through Accidental Degeneracy Caused by Lack of Symmetry, *J. Chem. Phys.*, 148, 204307 (2018).
217. Legesse, M.; Park, H.; El Mellouhi, F.; Kais, S.; et. al., Improved Photoactivity of Pyroxene Silicates by Cation Substitutions, *ChemPhysChem* 19, 943-953 (2018).
218. Friedrich, B; Herschbach, D; Kais, S; Schmidt, B., Molecules Enhanced by Electromagnetic Fields, *SciTech Europa, Quarterly*, 27 (2018).
219. Hu, Zixuan; Engel, Gregory; Alharbi, Fahhad; Kais, S., Dark States and Delocalization: Competing Effects of Quantum Coherence on the Efficiency of Light Harvesting Systems, *The Journal of Chemical Physics*, 148, 064304, (2018).
220. Hoehn, R.H.; Nichols, D.E.; Neven, H.; Kais, S., Status of the Vibrational Theory of Olfaction, *Frontiers in Physics*, 6,25 DOI: 10.3389/fphy.2018.00025 (2018).
221. Wei, Qi; Yasuikel, Tomokazu; Herschbachi, Dudley; Kais, Sabre
Pendular Alignment and Strong Chemical Binding are Induced in Helium Dimer Molecules by Intense Laser Fields, *PNAS*, 1-9 (2018).
222. Szczesniak, D., Hoehn, R.D., Kais, S.
“Canonical Schottky barrier heights of transition metal dichalcogenide monolayers in contact with a metal”, *Phys Rev B*,97,195315 (2018).

223. Wang, Dong; Shi, Wei-Nan; Hoehni, Ross; Kais, Sabre; et. al. Effects of Hawking Radiation on the Entropic Uncertainty in a Schwarzschild Space-Time *Ann.Phys. (Berlin)* 530, 1800080 DOI:10.1002/andp/201800080 (2018)
224. Rongxian Xia and Sabre Kais, "Quantum Machine Learning", *Nature Communications, Nature Comm.* 9, 4195 (2018).
225. Daskin, Ammar; Kais, Sabre, Direct Application of the Phase Estimation Algorithm to Find the Eigenvalues of the Hamiltonians, *Chemical Physics*, <https://doi.org/10.1016/j.chemphys.2018.01.002> (2018)
226. Daskin, Ammar; Kais, Sabre, A Generalized Circuit for the Hamiltonian Dynamics Through the Truncated Series, *Quantum Information Processing*, 17:328 (2018)
227. Wang, Dong; Hoehn, Ross; Kais, Sabre; et.al. Probing Entropic Uncertainty Relations Under a Two-atom System Coupled with Structured Bosonic Reservoirs *Quantum Information Processing*, 17:335 (2018).
228. Jiang, S.; Britt, K.; McCaskey, A.J.; Humble, T.; Kais, S., Quantum Annealing for Prime Factorization, *Scientific Reports* 8:17667 (2018).
229. Hu, Zixuan; Engel, Gregory; Kais, Sabre, Double-Excitation Manifold's Effect on Exciton Transfer Dynamics and the Efficiency of Coherent Light Harvesting, *Phys. Chem. Phys.* 20, 30032 (2018)
230. Massey, Sara; Ting, Po-Chieh; Yeh, Shu-Hao, Kais, Sabre; et. al. Orientational Dynamics of Transition Dipoles and Exciton Relaxation in LH2 from Ultrafast Two-Dimensional Anisotropy *J. Phys. Chem Lett.* 10, 270-277 (2019).
231. Fedwa El-Mellouhi, Sabre Kais, et. al.,"Enhancing the Electronic Dimensionality of Hybrid Organic-Inorganic Frameworks by Hydrogen Bonded Molecular Cations *Materials Horizons COMMUNICATION*, DOI:10.1039/c8mh01436a (2019).
232. Bian, T., Murphy, D., Xia, R., Daskin, A., Kais, S. Quantum Computing Methods for Electronic States of the Water Molecule *Molecular Physics*, DOI:10.1080/00268976.2019.1580392 (2019)
233. Hoehn, R.D., Francisco, J.S., Kachmar, A., "Role of Water on the Rotational Dynamics of the Organic Methylammonium Cation: A First Principles Analysis, *Scientific Report*, 9; 668, (2019).
234. Junxu Li, Sabre Kais, " Entanglement Classifier in Chemical" Reactions", *Science Advances* 5: 5283 (2019).
235. Yeh, SH, Hoehn, RD; Allodi, MA ; Engel, GS ; Kais, S. , "Elucidation of near-resonance vibronic coherence lifetimes by nonadiabatic electronic-vibrational state character mixing", *PNAS*, 116, 18263 (2019).
236. Daskin, Ammar; Bian, Teng; Xia, Rongxin; Kais, Sabre, " Content-Aware Quantum Simulation of a Matrix Stored in Quantum Memory" *Quantum Information Processing*, 18, 357, (2019).
237. Hsuan-Hao Lu, Wang, Yuchen; Weiner, Andrew; Kais, Sabre; "Quantum Phase Estimation with Time-Frequency Qudits in a Single Photon", *Adv: Quantum Technol.*, 1900074, (2019).

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 andMolecular 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).

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).

Invited Lectures

1. Harvard University, Department of Physics (Harvard Quantum Initiative) , "Quantum Machine Learning for Complex Systems", November 6, 2019.
2. 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.
3. DOE PIs meeting, "Quantum Computing Algorithms and Applications for Complex Chemical Systems", Gaithersburg Maryland, May 21-24, 2019.
4. Argonne National Lab, Quantum Information and Computation for Chemistry, Chicago, May 7, 2019.
5. Yale University , Quantum Information and Computation for Chemistry, , May 3, 2019.
6. International Symposium of Quantum Science and technology at Purdue, "Quantum Computing for Chemistry", April 21-23, 2019.
7. Purdue-IU Quantum workshop, "Quantum Algorithms for Chemistry, Feb. 26, 2019.
8. The 59th Sanibel Symposium "Quantum Computing for Complex Chemical Systems" Quantum Theory Project, University of Florida, February 17 - 22, 2019.
9. 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.
10. NSF "Quantum Computing Workshop", Nov. 7, 2018. Quantum Computing for chemistry.
11. NIST workshop on Complex Systems Chemistry, Gaithersburg, Maryland, "Quantum Information and Computing for Chemistry", October 22-24, 2018.
12. National Academies of Sciences, Engineering & Medicine, Chemical Sciences Roundtable, "Quantum Computing", Friday, July 27, 2018.
13. Israeli Academy of sciences, Quantum Machine Learning for Electronic Structure, June 18, 2018, Jerusalem.
14. Air Force Institute of Technology 2950 Hobson Way WPAFB OH, "Near term applications of small scale quantum computing for quantum chemistry", May 3, 2018.

15. IBM-Zurich, "Near term applications of small scale quantum computing for quantum chemistry", June 6, 2018.
16. "Cold molecules for chemistry" symposium at ACS Spring meeting, "Quantum computing with polar molecules", March 18-20 2018.
17. NASA, Lockheed-Martin center for Innovation, Suffolk, VA, Near term applications of small scale quantum computing for quantum chemistry, November 7, 2017.
18. Department of Chemistry, University of Chicago, Near term applications of small scale quantum computer", October 24, 2017.
19. 254th ACS Meeting, Mapping electronic structure Hamiltonian to an Ising type Hamiltonian , August 20-21, 2017.
20. Department of Physics, Purdue University, "Near term applications of small scale quantum computer", April 27, 2017.
21. APS, March Meeting 2017, Chairing the Session "Near term applications of small scale quantum Computing", New Orleans, March 13-17, 2017.
22. Department of Computer Science, Purdue University, "Near term applications of small scale quantum computer", February 27, 2017.
23. Department of Mathematics, Purdue University, "Near term applications of small scale quantum computer", February 10, 2017.
24. Wabash College, Department of Physics, Crawfordsville, IN 47933, "Near term applications of quantum computing", February 6, 2017.
25. Oak Ridge National Laboratory, Quantum Information and Computation: Second Quantum Technology Revolution, January 11, 2017.
26. Zurich IBM Research Laboratory, Adiabatic Quantum Computing, January 25, 2017.
27. 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.
28. Challenges of Electronic Structure Calculations on Quantum Computers, Department of Chemistry, Purdue University, November 16, 2016.
29. Freie Universität Berlin, Challenges of Electronic Structure calculations on Quantum Computers, October 4, 2016.
30. Department of Chemistry, University of Virginia, Quantum Information and Quantum Computation for Chemistry, September 30, 2016.
31. Department of Computer Engineering, Istanbul Medeniyet University, Kadikoy, Istanbul, Turkey, Light Matter Interaction: The role of quantum coherence, April 5, 2016.
32. Swiss Chemical Society, Fall Meeting 2015, Lausanne, Challenges of Electronic Structure Calculations, Sept. 4, 2015.
33. 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
34. KAUST, Saudi Arabia, "Light matter interactions", April 29, 2015.

35. Qatar Foundation, "New Challenges for Electronic Structure calculations", April 13, 2015.
36. Swiss Chemical Society, Fall Meeting 2014, Zurich, Light Matter Interaction, Sept. 11, 2014.
37. IBM Zurich, Switzerland, Challenges of Electronic Structure Calculations for Atoms and Molecules, Zurich, Switzerland, Feb. 26, 2014.
38. Laboratory of Physical Chemistry, ETH, Quantum Coherence and Light matter Interaction, ETH, Zurich, Switzerland, Feb. 27, 2014.
39. Physics and Engineering ICube Laboratory/CNRS, University of Strasbourg, Light Matter Interaction : The role of quantum coherence, Strasbourg, France, Feb. 24, 2014
40. State Key Laboratory of Precision Spectroscopy East China Normal University, Challenges of Electronic Structure Calculations for Atoms and Molecules", Shanghai, China Dec. 1, 2013.
41. China Academy of Engineering Physics, Light Matter Interaction, Mianyang, China Dec. 3, 2013
42. China Academy of Engineering Physics, The Role of Quantum Coherence in Different Systems , Mianyang, Dec. 4, 2013
43. Sigma Xi Award Lecture, Quantum Information for Quantum Chemistry, Purdue, March 25, 2013.
44. 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
45. APS March Meeting 2013, March 18 - March 22, Baltimore, Maryland Tutorial 4 Quantum Information and Computation for Quantum Chemistry.
46. Santa Fe Institute, Quantum Coherence and Entanglement in Complex Systems, April 6, 2012.
47. Los Alamos National Lab, Quantum Entanglement, April 5, 2012.
48. Quantum Computation for Quantum Chemistry: Status, Challenges, and Prospects, Microsoft Research Redmond, Nov, 12, 2012, Redmond, WA
49. Winter School 2012, Quantum Information and Computation for Quantum Chemistry, January 5-7, 2012 at Indian Wells, CA

50. Banff Meeting, BIRS workshop on Quantum Information for Quantum Chemistry, June 6-11, 2011, Banff, Canada.
51. 241st ACS meeting, Division of Physical Chemistry, Anaheim, CA, Tuning and Quenching Entanglement of Dipole Arrays, March 30, 2011
52. Computer Science Department, Purdue University, Quantum Information and Quantum Computation, March 9, 2011.
53. 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.
54. King Abdullah Institute for Nanotechnology, Riyadh, Saudi Arabia, Research Projects in Birck Nanotechnology Center at Purdue, December 20, 2010.

55. Department of Physics (Malaz), King Saud University, Riyadh, Saudi Arabia, Quantum Information and Quantum Computation: Toward Realizing a Quantum Computer, December, 21 2010.
56. Department of Physics, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia, Finite Size Scaling, December 25, 2010.
57. Department of Physics, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia, Quantum Information and Computation, December 26, 2010.
58. Department of Physics, East China Normal University, China, Finite Size Scaling and Quantum Criticality, November 25, 2010.
59. Chinese Academy of Engineering Physics, Mianyang, China, Stability of Atomic and Molecular Systems in Superintense Laser Fields, November 26, 2010.
60. Purdue University, Computer Science, ``Quantum Information and Quantum Computation'', October 6, 2010.
61. TMAU-Princeton Summer Workshop on Quantum Optics and Molecular Physics, Quantum Information for Quantum Chemistry\ Casper, Wyoming, July 25-31, 2010.
62. 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.
63. 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.
64. Chair: 42nd Midwest Theoretical Chemistry Conference, Department of Chemistry, Purdue, May 20-22, 2010.
65. Department of Physics, Purdue, Quantum Information for Quantum Chemistry", February 11, 2010.
66. The 41st Midwest Theoretical Chemistry Conference, ``Finite Size Scaling and Quantum Criticality'', Southern Illinois University, Carbondale Illinois, May 28-30, 2009.
67. Rutgers University, THE 101ST STATISTICAL MECHANICS CONFERENCE, ``Finite Size Scaling in Quantum Mechanics'', SUNDAY - TUESDAY, MAY 10-12, 2009.
68. 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.
69. Fritz Haber Institute of the Max Planck Society, Department of Molecular Physics, Berlin, Germany" Finite Size Scaling and Quantum Criticality", December 12, 2008.
70. Ruhr University, Institute for Theoretical Chemistry, Bochum, Germany" Finite Size Scaling and Quantum Criticality", December 3, 2008.
71. 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.
72. 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.
73. University of Heidelberg, Institute for Theoretical Chemistry, Universitaet Heidelberg, Germany," Finite Size Scaling and Quantum Criticality", October 20, 2008.
 74. Freie Universitaet Berlin, Department of Chemistry, Berlin, Germany" Finite Size Scaling in Quantum Mechanics", September 10, 2008.
 75. Max Planck Institute for Physics of Complex Systems, Dresden, Germany" Quantum Criticality", August 22, 2008.
 76. University of Chicago, James Franck Institute (JFI), "Suppose We Build a Quantum Computer, How Chemistry Can Benefit From Such a Computer", June 10, 2008.
 77. Santa Fe Institute, ``Finite Size Scaling and Quantum Criticality'', February 7, 2008.
 78. Harvard-MIT-BU-BC Theory Seminar, ``Finite Size Scaling in Quantum Mechanics'', November 26, 2007.
 79. Purdue University, Electrical and Computer Engineering, Nano501 ``Finite Size Scaling and Quantum Criticality'', November 12, 2007.
 80. Illinois Institute of Technology, Physical Sciences, `` Finite Size Scaling for Atomic and Molecular Systems'', October 25, 2007.
 81. Illinois Institute of Technology, Chemical Engineering, `` Quantum Phase Transition and Stability of Atomic and Molecular Systems'', September 5, 2007
 82. Technion-Israel, Department of Chemistry, ``Finite Size Scaling in Quantum Mechanics'', June 24, 2007.
 83. Lewiner Institute of Theoretical Physics, Technion-Israel, Correlated Electrons Day, ``Finite Size Scaling in Quantum Mechanics'', June 21, 2007.
 84. Yarmouk University, Jordan, ``Quantum Phase Transition and Stability of Atomic and Molecular Systems'', May 29, 2007.
 85. 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"
 86. Princeton-TAMU Foundations of Quantum Mechanics Symposium, ``Dimensional Scaling for Stability of Atomic and Molecular Systems'', Princeton, 16-17 February 2007.
 87. Department of Chemistry, Purdue University, West Lafayette "Finite Size Scaling for Stability of Atomic and Molecular Systems", February 7, 2007.
 88. 38th Midwest Chemistry Conference, 'Entanglement and electron Correlation in Quantum Chemistry calculations", Ohio State University Campus, Columbus Ohio, June 15-17, 2006
 89. The 36th Winter Colloquium on the Physics of Quantum Electronics," Entanglement as a measure of electron-electron correlation", Snowbird, Utah, January 2-6, 2006.
 90. 230th ACS meeting, Washington DC, Aug. 28-Sept. 1, 2005, "Finite Size Scaling for Critical Phenomena in Negative Ion Clusters"
 91. Casper College-Texas A M University Quantum Optics Summer Workshop, August 14-August 20, 2005, "Finite Size Scaling in Quantum Mechanics"

92. 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"
93. Stanford University, CA, Department of Chemistry, June, 23, 2005, "Finite Size Scaling in Quantum Mechanics"
94. Purdue University, Computer Science and Engineering Spring 2005 Seminar Series, April 27, 2005 "Quantum Computing"
95. Department of Chemistry, Purdue University, West Lafayette "Finite Size Scaling in Quantum Mechanics", March 9, 2005.
96. 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"
97. Department of Chemistry, Technion Haifa 32000, Israel, July 27, 2004 "Tuning the Entanglement for magnetic Systems"
98. Department of Chemistry, Technion Haifa 32000, Israel, July 25, 2004 "Finite Size Scaling and Stability of Atomic and Molecular Ions"
99. Department of Chemistry, Purdue University, West Lafayette "Finite Size Scaling in Quantum Mechanics", March 24, 2004.
100. Kansas State University, Department of Chemistry Manhattan KS 66506-3701, "Finite Size Scaling for Stability of Atomic and Molecular Systems", March 18, 2004
101. WISICT 2004, Winter International Symposium on Information and Communication Technologies, Cancun, Mexico, January 5th-8th, 2004 "Scaling of Entanglement at Quantum Phase Transitions"
102. WISICT 2004, Winter International Symposium on Information and Communication Technologies, Cancun, Mexico, January 5th-8th, 2004 Chair: Workshop on Quantum Information Processing
103. Department of Mathematics, Purdue University, West Lafayette "Finite Size Scaling in Quantum Mechanics", October 3, 2003.
104. NASA JET PROPULSION LABORATORY, California Institute of Technology, "Scaling of Entanglement at Quantum Phase Transitions", August 15, 2003.
105. Workshop on Quantum Computing, "Tuning the Entanglement for magnetic Systems", University of Notre Dame, Notre Dame, IN, August 7, 2003
106. 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"
107. 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)
108. Florida State University, Department of Chemistry, "Quantum Critical Phenomena and Stability of Atomic and Molecular Ions" (invited by Prof. Sanford Safran)
109. The University of British Columbia, Department of Chemistry, Vancouver, Canada, June 10, 2002 "Finite Size Scaling and Renormalization Group for Quantum Critical Phenomena"

110. 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"
111. 2002 DAMOP Annual Meeting, May 29-June 1 Williamsburg, VA meeting of the "Finite Size Scaling for Atomic and Molecular Systems"
112. University of Wisconsin-Madison, Department of Chemistry, Madison, WI, May 20, 2002, "Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
113. ONR Program Review, Arlington, Virginia, April 30- May 3, 2002"Critical Phenomena and Renormalization Group Approach for Electronic Structure calculations"
114. Yale University, Department of Physics, New Haven, CT, April 22, 2002 "Finite Size Scaling for Quantum Critical Phenomena"
115. Carnegie Mellon University, Department of Chemistry, Pittsburgh, Pennsylvania, April 11, 2002."Quantum phase transitions and Stability of atomic and molecular systems"
116. APS March Meeting 2002, Indianapolis, IN, March 18, 2002Session A31 (Chemical Physics of Complex Systems)"Finite Size Scaling in Quantum Mechanics"
117. APS March Meeting 2002, Indianapolis, IN, March 20, 2002Session M20 (One Dimensional Theory)"Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
118. Sanibel Symposium 2002 in Quantum Chemistry, Florida, February 23, 2002, Chair of plenary session on Multi-Scale Simulation.
119. Illinois Institute of Technology, Department of Biological, Chemical and Physical Sciences, Chicago, IL, February 20, 2002"Finite Size Scaling for Quantum Critical Phenomena"
120. Purdue University, CS& E Spring 2002 Seminar Series, February 13, 2002 "Finite Size Scaling for Quantum Critical Phenomena"
121. Department of Chemistry, University of Michigan, Ann Arbor, MI, November 8, 2001"Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
122. Department of Chemistry, Wayne State University, Detroit, MI, November 7, 2001"Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
123. Department of Chemistry, Rutgers University, Piscataway, NJ, June 19, 2001"Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
124. Sanibel Symposium 2001 in Quantum Chemistry Florida, February 28, 2001"Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
125. Purdue University, Department of Chemistry West Lafayette, IN, January 17, 2000 "Quantum Phase Transitions and Stability of Atomic and Molecular Ions".
126. Department of Chemistry, Hebrew University, Jerusalem Israel, November 28, 2000"Quantum Phase Transitions and Stability of Atomic and Molecular Systems"

127. Department of Chemistry, Ben Guroun University, Israel November 15, 2000"Quantum Phase Transitions and Stability of Atomic and Molecular Systems"
128. Advances in Finite Time Thermodynamics, Jerusalem, Israel November 12-14, 2000"Quantum Phase Transitions at $T=0$ ".
129. 2000 Midwest Thermodynamics and Statistical Mechanics Conference, Minneapolis, Minnesota, May 14-16, 2000."Finite Size Scaling for Critical Parameter of Simple Diatomic Molecules"
130. Department of Chemistry, Wabash College, Crawfordsville, IN 47933, Tuesday Feb. 29, 2000 "Recent Advances in Electronic Structure Theory".
131. Department of Chemistry, Indiana University Bloomington, Indiana 47405, Thursday, September 23, 1999"Phase Transitions and Stability of Atomic and Molecular Ions."
132. Department of Chemistry and Physics, Indiana University, Bloomington, Indiana 47405, Friday, September 24, 1999"Finite Size Scaling in Quantum Mechanics".
133. Technion, Department of Chemistry Haifa 32000, Israel, Sunday June 13, 1999 "Recent Advances in Density Functional Theory".
134. The Ohio State University Department of Chemistry Columbus, OH 43210, Monday, April 26, 1999"Phase Transitions and Stability of Atomic and Molecular Ions".
135. Purdue University, Department of Physics, West Lafayette, IN, January 29, 1999 "Phase Transitions and Stability of Atomic and Molecular Ions".
136. University of Illinois at Urbana-Champaign, Department of Chemistry Urbana, IL, December 2, 1998"Phase Transitions and the Stability of Atomic and Molecular Ions".
137. Purdue University, Department of Chemistry West Lafayette, IN, September 7, 1998 "Phase Transitions and Stability of Atoms and Molecules".
138. 31st Midwest Theoretical Chemistry Conference Department of Chemistry, Purdue University Chair of the Conference.
139. University of California UCLA, Department of Chemistry Los Angeles, CA, March 11, 1998 "Phase Transitions and Stability of Atoms and Molecules".
140. The American Physical Society - 1998 March Meeting, Los Angeles, CA 16-20 March, 1998" Phase Transitions and Stability of Atomic and Molecular Negative Ions".
141. Southern Methodist University Department of Chemistry Dallas, Texas, April 23, 1998" Phase Transitions and Stability of Atoms and Molecules".
142. Hebrew University, Department of Chemistry Jerusalem, Israel, December 22, 1997 "Phase Transitions and Stability of Atoms and Molecules".
143. Technion, Department of Chemistry Haifa, Israel, December 23, 1997 "Phase Transitions and Stability of Atoms and Molecules".
144. 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".
145. 30th Midwest Theoretical Chemistry Conference University of Illinois, Urbana-Champaign, May 22-24, 1997 "Comparison of Pivot Methods for Global Optimization"

146. The American Physical Society - 1997 March Meeting Kansas City, MO 17-21 March, 1997 "A New Approach for Global Optimization".
147. 29th Midwest Theoretical Chemistry Conference Indiana University-Purdue University Indianapolis, May 30- June 1, 1996" A New Approach to Global Minimization".
148. The American Physical Society: Atomic, Molecular and Optical Physics Indianapolis, Indiana, April 2, 1996"Critical Phenomena for Electronic Structure at the Large-D limit".
149. The University of Illinois at Chicago Department of Chemistry Chicago, Illinois, March 7, 1996 "Dimensional Renormalization for the Treatment of Electron Correlation".
150. Purdue University: The Dean's Freshman Honors Seminar (SCI 110), Nov. 20, 1995 "New Challenges in Quantum Chemistry".
151. 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".
152. Technion, Physics Department Haifa, Israel, June 13, 1995 "Dimensional Renormalization for Electronic Structure of Atoms and Molecules".
153. Regensburg University, Institute for Theoretical Chemistry Regensburg, Germany, May 22, 1995"Dimensional Renormalization for Electronic Structure of Atoms and Molecules".
154. NATO Advanced Research Workshop on New Methods in Quantum Theory Halkidiki, Greece, May 14-19, 1995 "Dimensional Renormalization for Electronic Structure Calculations".
155. Northwestern University, XXVIII Midwest Theoretical Chemistry Conference Evanston, Illinois, May 11-13, 1995 "Charge Renormalization at the Large-D Limit for Electronic Structure Calculations".
156. Purdue University, Department of Physics West Lafayette, IN March 20, 1995 Molecules and Clusters".
157. Oregon State University, Department of Chemistry Corvallis, Oregon, April 14, 1993"Electronic Structure Calculations by Density Functional Theory and Dimensional Scaling Methods".
158. Harvard University, Dudley Herschbach's 60th Birthday Cambridge, MA, July 1992 "Dimensional Scaling the Quasi stationary States".
159. Cambridge University, Department of Chemistry Cambridge, England, June 1992"Electronic Structure Calculations by Density Functional and Dimensional Scaling".
160. Cornell University, Department of Physics Ithaca, NY, March 3, 1992"Electronic Structure Calculations by Density Functional and Dimensional Scaling".
161. M.I.T., Department of Chemistry Cambridge, MA, October 30, 1991"Tunneling in Multi-Dimensional Systems".
162. New York University, Department of Physics New York, New York, October 21, 1991"Dimensional Scaling Method in Atomic and Molecular Physics".
163. Orsted Institute, Department of Chemistry Copenhagen, Denmark, June 1991Conference in Dimensional Scaling in Chemical Physics "Symmetry Breaking and Electronic Exchange Energy".

Other Presented Papers

- 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 (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, 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 1995 Poster: Charge Renormalization at the Large-D Limit for Electronic Structure Calculations.
- Northwestern University, XXVIII Midwest Theoretical Chemistry Conference Evanston, Illinois, May 11-13, 1995 Poster: Charge Renormalization at the Large-D Limit for Electronic Structure Calculations.
- Sanibel Symposium in Quantum Chemistry Florida, February 25 - March 4, 1995 Poster: 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, 1991 Hidden Crossings in Ion-Atom Collisions and in Other Nonadiabatic Transitions.