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PROFESSIONAL ADDRESS

Division of Advanced Cyberinfrastructure
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EDUCATION

- Brooklyn College BS/Chemistry, 1962 Cum Laude, honors in chemistry
- Yale University MS/Chemistry, 1964
- The University of Chicago Ph.D, Theoretical Chemistry, 1968
Thesis Advisor: Professor R. Stephen Berry
- The University of Southern California Postdoctoral Fellow
Post-doctoral Advisor: Professor Howard S. Taylor

PROFESSIONAL EXPERIENCE

- General Telephone and Electronics Laboratory 1969-1972
- Research in Atomic and Molecular Physics related to advanced lighting sources
 - Technological Forecasting
- Theoretical Division, Los Alamos National Laboratory 1972 - 1991
- Theoretical Chemistry and Physics
 - Quantum Chemistry
 - Atomic and Molecular scattering processes
 - Numerical Methods
 - Computational Physics
- Physics Division, National Science Foundation 1991 - 2009
- Program Director, Theoretical Atomic, Molecular, and Optical Physics

- ▷ Budget of \$4.4M/Yr
 - Program Director, Physics at the Information Frontier
 - ▷ Budget of \$9.5M/Yr
 - Program Director, Plasma Physics
 - ▷ Budget of \$6.0M/Yr
- Office of Cyberinfrastructure/Division of Advanced Cyberinfrastructure, National Science Foundation
2009 - Present
- Program Director, eXtreme Science and Engineering Discovery Environment (XSEDE) 2009-2012
 - ▷ Budget of \$25M/Yr
 - Program Director, eXtreme Digital Project including all Track 2 Resources
 - ▷ Total Budget of \approx \$250M

ADDITIONAL POSITIONS

NIST, Guest Research Scientist	1995-present
NIST, Sabbatical Leave	2000-2001
Poste Rouge, CNRS, Observatoire de Paris, France	1980
Humboldt Award, University of Kaiserslautern	1987

HONORS AND AWARDS

Elected Fellow of American Physical Society	1983
<ul style="list-style-type: none"> • Cited for seminal research in applications of many-body theory to atomic and molecular collisions 	
Humboldt Prize of German Government	1987-1988
<ul style="list-style-type: none"> • In recognition of theoretical and computational research in electron-molecule collisions 	
Poste Rouge/CNRS	1979-1980
<ul style="list-style-type: none"> • Research in electron-molecule collisions 	
NSF Directors Award for Collaborative Integration	1997-1998
<ul style="list-style-type: none"> • NSF/DoE Plasma Science and Engineering Initiative 	

PROFESSIONAL EXPERIENCE

- Co-organizer of West Coast Theoretical Chemistry Conference, 1975
- Instructor, Los Alamos Summer School For Atomic Physics, 1989-97
- High Performance Computing and Communications Coordinator, Physics Division - National Science Foundation, 1993
- Grand Challenge Coordinator MPS Directorate - National Science Foundation, 1993
- Review Board-Cornell Supercomputer Center, 1992-1997
- Proposal Processing Committee for MPS Directorate - National Science Foundation, 1994
- MPS Committee to investigate Basic Assumptions of NSF/Researcher/University/Congressional Interactions -National Science Foundation, 1994
- Chairman, Interagency Committee for Atomic, Molecular and Optical Science, 1993-1994
- Grand Challenge Coordinator for Interdisciplinary Activities - MPS Directorate - National Science Foundation, 1995.
- Optical Science and Engineering Working Group - National Science Foundation, 1996
- Chairman, National Science Foundation Plasma Science and Engineering Working Group, 1996-97
- Chairman, NSF/DoE Partnership in Basic Plasma Science and Engineering, 1997-1998
- APS Davisson-Germer Prize Selection Committee, 1998
- Vice-Chair and Chair-Elect APS Few-Body Topical Group, 1997-1999
- Chair, APS Few-Body Topical Group, 2000
- Visiting Scientist, National Institute of Standards and Technology, 1995-present
- Visiting Scientist, Theoretical Division, Los Alamos National Laboratory, 1991-present

- Organizer of workshop, Computational Methods for Few-Body Dynamical Problems, NIST, 2000
- Chairman, MPS Directorate, Information Technology Working Group, 2001-2002
- Chairman, Scientific Frontiers Working Group for Information Technology Initiative, 2001-2002
- Chairman, NSF/DoE Partnership in Basic Plasma Science and Engineering, 2001-2002
- Organizer, NSF workshop, Computation as a Tool for Discovery in Physics, 2001
- Reviewer of Computational Science Division, Daresbury Laboratory for EPSRC, 2002 and 2005
- MPS representative to NSF Cyberinfrastructure Working Group, 2003-2004
- Vice-Chair and Chair Elect, APS Division of Computational Physics, 2002-2003
- Chair, APS Division of Computational Physics, 2004-2005
- Program Chair, Conference in Computational Physics, 2005
- Internal Liaison, Grand Challenge Communities, 2009-2010
- Vice-Chair and Chair Elect, APS Division of Computational Physics, 2013-2014
- Editor, Computers in Science and Engineering, 2012-present
- Program Committee, Conference in Computational Physics, 2014

PROFESSIONAL INTERESTS

- Theoretical Chemistry and Physics
- Atomic and Molecular Physics
 - Theory of scattering processes
 - Photoionization
 - Interaction of strong, short pulse radiation with atoms and molecules
- Applications of many-body theory to atomic and molecular systems
- Quantum Chemistry
 - Calculation of the potential curves of ground and excited states of diatomic molecules
 - Electron correlation
 - Electron affinities of molecular ions
 - Molecular polarizabilities
- Applications of Pseudo-Potentials to molecular systems
- Applications of large-scale computers to physics and chemistry
 - Development of computer codes adapted to vector and parallel Processors
- Numerical Analysis
 - Solution of integral equations
 - Iterative methods for linear systems
 - Eigenvalue problems
 - Special functions
 - Time-dependent propagation methods

POSTDOCTORAL ASSOCIATES

- Professor Michael Morrison
Department of Physics and Astronomy
The University of Oklahoma
Norman, Oklahoma
- Dr Diane Lynch
Department of Chemistry and Biochemistry
Kennesaw State University
Kennesaw, GA
- Professor David Feder
Department of Physics
University of Calgary
Calgary CA
- Professor Nicolai Nygaard
Aarhus University
Aarhus, Denmark
- Dr Johannes Feist
Institute for Theoretical Atomic and Molecular Physics
Harvard-Smithsonian
Cambridge, MA

PROFESSIONAL SOCIETIES

- American Physical Society
 - Division of Atomic, Molecular and Optical Physics
 - Division of Chemical Physics
 - Division of Computational Physics
 - Few Body Topical Group
- American Chemical Society

INTERESTS and ACTIVITIES

Music of all types, especially classical music and the vocal and operatic repertoire, running and guitar playing

PUBLICATIONS [Over 4000 Citations;H-Index 36]

1. B. I. Schneider, M.C. Weinberg, J. C. Tully and R. S. Berry, Pseudopotential Method for Inelastic Processes in Atoms and Molecules. I. General Method and Photodetachment of O^- Phys. Rev., **182**, 133 (1969)
2. B.I. Schneider and R.S. Berry, Pseudopotential Method for Inelastic Process in Atoms and Molecules. II. Photoionization of N_2 , Phys. Rev. **182**, 141 (1969).
3. B. I. Schneider and R. S. Berry, Photoionization of Molecules: Pseudopotential Theory, Recent Developments in Mass Spectroscopy, K. Ogata and T. Hayakawa, editors, University of Tokyo Press (1970).
4. B.I. Schneider, H.S. Taylor and R. Yaris, Many-Body Theory of the Elastic Scattering of Electrons from Atoms and Molecules, Phys. Rev. **A1**, 855 (1970).
5. B.I. Schneider, Inelastic Scattering of High Energy Electrons from Atoms: The Helium Atom, Phys. Rev. **A2**, 1873 (1970).
6. B.I. Schneider, Low Energy Scattering in the Random Phase Approximation, Phys. Rev. **A4**, 1008 (1971).

7. H.S. Taylor, B.I. Schneider, R. Yaris, and B.S. Yarlagadda, Applications of Many-Body Green's Function Theory to Helium, *Phys. Rev.* **A7**, 146 (1973).
8. B.I. Schneider, Green's Function Theory of Photoionization, *Phys. Rev.* **A7**, 557 (1973).
9. B.I. Schneider, Study of the Potential Curves of Xenon with Other Rare Gas Atoms, *J. Chem. Phys.* **55**, 4447 (1973).
10. B.I. Schneider, H.S. Taylor and R. Yaris, Initial Effective Potentials Derived from Many-Body Green's Function Theory: Application to Lithium, *Chem. Phys. Lett.* **22**, 381 (1973).
11. B.I. Schneider, The Use of Gaussian Basis Functions in Fredholm Calculations of Electron-Atom and Electron-Molecule Collisions, *Chem. Phys. Lett.* **25**, 140 (1974).
12. B.I. Schneider and J.S. Cohen, Potential Curves, Radiative Processes and Resonant Energy Transfer Cross Sections in Ne, *Rad. Res.* **59**, 363 (1974).
13. B.I. Schneider, Interaction Potentials for UF₆ with Itself and with Rare-Gas Atoms, *Chem. Phys. Lett.* **27**, 577 (1974).
14. B.I. Schneider and J.S. Cohen, Ground and Excited States of Ne₂ and Ne₂⁺. I. Potential Curves with and without Spin-Orbit Coupling, *J. Chem. Phys.* **61**, 3230 (1974).
15. B.I. Schneider and J.S. Cohen, Ground and Excited States of Ne₂ and Ne₂⁺: Spectroscopic Properties and Radiative Lifetimes, *Chem. Phys.* **61**, 3240 (1974).
16. B.I. Schneider and J.S. Cohen, Collisions of Ne* (3s) and Ne⁺ with Ne: Excitation and Charge Transfer, Elastic Scattering and Diffusion, *Phys. Rev.* **A11**, 884 (1975).
17. B.I. Schneider, R-Matrix Theory of Electron-Molecule Scattering Using Analytic Basis Set Expansions, *Chem. Phys. Lett.* **31**, 237 (1975).
18. B.I. Schneider, R-Matrix Theory of Electron-Molecule Scattering Using Analytic Basis Set Expansions. II. Electron H₂ Scattering in the Static-Exchange Model, *Phys. Rev.* **A11**, 1957 (1975).
19. P.J. Hay and B.I. Schneider, Elastic Scattering of Electrons from F₂, *J. Phys.* **B9**, 1165 (1976).
20. P.J. Hay and B.I. Schneider, Elastic Scattering of Electrons from F₂: An R-Matrix Calculation, *Phys. Rev.* **A13**, 2049 (1976).
21. B.I. Schneider, Role of the Born-Oppenheimer Approximation in the Vibrational Excitation of Molecules by Electrons, *Phys. Rev.* **A14**, 1923 (1976).
22. B.I. Schneider and M.A. Morrison, Elastic Scattering of Electrons from N₂: An R-Matrix Calculation, *Phys. Rev.* **A16**, 1003 (1977).
23. B.I. Schneider, Pseudostates and Low Energy Electron-Molecule Collisions: Applications to H₂ and N₂, *Chem. Phys. Lett.* **51**, 578 (1977).
24. B.I. Schneider, The R-Matrix Method: Applications to Electron Molecule Collisions, invited lecture and paper in *Electronic and Atomic Collisions: Proceedings of the 10th International Conference on the Physics of Electronic and Atomic Collisions, Paris, 21-27 July, 1977*, edited by G. Watel, pp. 257-269 (1977).
25. B.I. Schneider, Theoretical Atomic and Molecular Physics at X ICPEAC, *Comments At. and Mol. Phys.*, **7**, 157 (1977).
26. B.I. Schneider and C.A. Brau, Dissociative Attachment of Electrons to F₂, *Appl. Phys. Lett.* **23**, 569 (1978).
27. B.I. Schneider and R.B. Walker, The Coupled Channel R-Matrix Propagation Method, *J. Chem. Phys.* **70**, 2466 (1979).
28. B. I. Schneider, *The R-Matrix Method for Electron-Molecule Scattering: Theory and Computation, Electron-Molecule and Photon-Molecule Collisions*, edited by Thomas Rescigno, Vincent McKoy and Barry Schneider, Plenum Press, New York and London, 1979
29. B.I. Schneider, M. LeDourneuf and P.G. Burke, Theory of Vibrational Excitation and Dissociative Attachment: An R-Matrix Approach, *J. Phys.* **B12**, 1365 (1979).

30. B.I. Schneider, M. LeDourneuf and Vo Ky Lan, Resonant Vibrational Excitation of N₂ by Low Energy Electrons: An Ab Initio R-Matrix Calculation, *Phys. Rev. Lett.* **43**, 1926 (1979).
31. Vo Ky Lan, M. LeDourneuf and B. I. Schneider, Rotational Excitation of Diatomic Polar Molecules by Slow Electrons; Practical Implementation of the Frame Transformation Theory, Book of invited papers, Proceedings of XI ICPEAC, 1979, North-Holland Publishing Company, New York, NY.
32. Vo Ky Lan, M. LeDourneuf and, B. I. Schneider, Comparative Merits of New Methods for Solving Local Coupled Channel Scattering Equations: The Variable Phase, R-Matrix Propagator, and Gailitis Expansion Method, Book of invited papers, Proceedings of XI ICPEAC, 1979, North-Holland Publishing Company, New York, NY.
33. B. I. Schneider, M. LeDourneuf and Vo Ky Lan, Vibrational Excitation of N₂ Using The R-Matrix Method, Book of invited papers, Proceedings of XI ICPEAC, 1979, North-Holland Publishing Company, New York, NY.
34. B.I. Schneider, Direct Calculation of Resonant Energies and Widths Using an R-Matrix Approach, *Phys. Rev.* **A24**, 1 (1981).
35. B.I. Schneider and L.A. Collins, A Linear Algebraic Approach to Electron Molecule Collisions, *J. Phys. B* **14**, 1101 (1981).
36. B.I. Schneider and L.A. Collins, A Linear Algebraic Method for Electron Atom/Molecule Collisions, II. Separable Exchange Potentials, *Phys. Rev.* **A24**, 1264 (1981).
37. B.I. Schneider and L.A. Collins, Linear Algebraic Method for Electron Atom/Molecule Collisions. Theory and Applications, *Phys. Rev.* **A24**, 2387 (1981).
38. B.I. Schneider and H.S. Taylor, The Solution of Driven Equations by R-Matrix Propagation Methods, *J. Chem. Phys.* **77**, 379 (1982).
39. B.I. Schneider and L.A. Collins, Application of Ab Initio Optical Potentials to Low Energy Electron-H₂ Scattering, *J. Phys. B* **15**, 1335 (1982).
40. B.I. Schneider and C.A. Brau, Two and Three Body Electron Attachment in Air, *J. Phys. B* **15**, 1601 (1982).
41. B.I. Schneider and L.A. Collins, Ab Initio Optical Potentials Applied to e+H₂ and e+N₂ in the Linear Algebraic Approach, *Phys. Rev.* **A27**, 2847 (1983).
42. B.I. Schneider and L.A. Collins, Examination of ¹Σ_g Resonances in Low Energy e+H₂⁺, *Phys. Rev.* **A28**, 166 (1983).
43. B.I. Schneider, M.G. Sheppard and R.L. Martin, Multi-Reference Many-Body Perturbation Theory: Application to O₂ Potential Energy Surfaces, *J. Chem. Phys.* **79**, 1364 (1983).
44. B.I. Schneider and L.A. Collins, Linear Algebraic Approach to Electron Molecule Collisions, Electron Molecule Collisions and Photoionization Processes: Proceedings of the First United States-Japan Seminar on Electron-Molecule Collisions and Photoionization Processes, p203, edited by Vincent McKoy, Hiroshi Suzuki, Kazuo Takayanagi, and Sandor Trajmar, Verlag Chemie International, Deerfield Beach, Florida, 1983
45. B. I. Schneider, R-Matrix Theory of Electron-Molecule Scattering, Electron-Atom and Electron-Molecule Collisions, p121, edited by Juergen Hinze, Plenum Press, New York, 1983.
46. M. LeDourneuf, Vo Ky Lan, and B. I. Schneider, Applications of R-Matrix and Frame Transformation Techniques to Vibrational and Rotational Excitation of Molecules, p135, edited by Juergen Hinze, Plenum Press, New York, 1983.
47. B.I. Schneider and L.A. Collins, Polarization and Correlation in Low Energy Electron Molecule Collisions, Proceedings of International Symposium on Wavefunctions and Mechanism in Electron Scattering Processes, ed. By F.A. Gianturco and G. Stefani, Springer Verlag 1984.
48. L.A. Collins and B.I. Schneider, Molecular Photoionization in the Linear Algebraic Approach: H₂, N₂, NO and CO₂, *Phys. Rev.* **A29**, 1695 (1984).

49. B.I. Schneider and L.A. Collins, Comparative Study of Low Energy Scattering on N₂, *Phys. Rev.* **A30**, 95 (1984).
50. L.A. Collins and B.I. Schneider, Separable Expansions in the Inelastic Scattering of Electrons from Atoms and Molecules, *J. Phys. B* **17**, 1235 (1984).
51. B.I. Schneider and L.A. Collins, Resonances in Electron Molecule Scattering and Photoionization, in American Chemical Society Symposium Series 263, Resonances in Electron-Molecule Scattering, van der Waals Complexes, and Reactive Chemical Dynamics, edited. By Donald G. Truhlar, American Chemical Society, Washington, DC, 1984, pp. 65-88.
52. B.I. Schneider, Applications of Projection Methods to Scattering Calculations, *Phys. Rev.* **A4**, 2188 (1985).
53. N.T. Padial, L.A. Collins and B.I. Schneider, Photoionization of C₂, *The Astrophysical Journal*, **298**, 369 (1985).
54. B.I. Schneider and L.A. Collins, Electronic Excitation of the b³Σ_u⁺ State of H₂, *J. Phys. B* **18**, L857 (1985).
55. B.I. Schneider and L.A. Collins, Application of the Linear Algebraic Method to Electronically Inelastic Collisions, *Phys. Rev.* **A33**, 2982 (1986).
56. B.I. Schneider and L.A. Collins, An Iteration-Variation Method for Scattering Problems, *Phys. Rev.* **A33**, 2970 (1986).
57. L.A. Collins and B.I. Schneider, Separable Expansions for Exchange Potentials in Inelastic Electronic Collisions, *Phys. Rev.* **A34**, 1564 (1986).
58. L.A. Collins, B.I. Schneider, C.W. McCurdy, S. Yabushita, and C.J. Noble, Curve Crossings in the ¹Π_u Autoionizing States of H₂: A Breakdown of the Traditional Independent Resonance Model, *Phys. Rev. Lett.* **57**, 980 (1986).
59. C.W. McCurdy, T.N. Rescigno and B.I. Schneider, On the Interrelation Between Variational Principles for Scattering and Generalized R-Matrix Theory, *Phys. Rev.* **A36**, 2061 (1987).
60. T.N. Rescigno and B.I. Schneider, Disappearance of Continuum Exchange Integrals from Algebraic Variational Calculations of Electron Scattering, *Phys. Rev.* **A37**, 1044 (1987).
61. D.L. Lynch, B.I. Schneider and T.A. Gibson, Comparison of Exact and Model Polarization Potentials for Electron-H Scattering, *Phys. Rev.* **A37**, 3590 (1988).
62. B.I. Schneider and T.N. Rescigno, Applications of the Complex Kohn Method to Inelastic e+H₂ Collisions, *Phys. Rev.* **A37**, 3749 (1988).
63. D.L. Lynch, B.I. Schneider, L.A. Collins, V. McKoy and W.M. Huo, Vibrationally Resolved Studies of the ²Π Photoionization of NO, *Chem. Phys. Lett.* **147**, 529 (1988)
64. D.L. Lynch, B.I. Schneider and L.A. Collins, Interaction of Shape, Valence and Autoionizing Resonances in NO, *Phys. Rev.* **A38**, 4927 (1988).
65. L.A. Collins and B.I. Schneider, Recent Advances in the Theory of Electron Impact Excitation of Molecules, *Electronic and Atomic Collisions: Invited Papers of the XV International Conference on the Physics of Electronic and Atomic Collisions*, Brighton, United Kingdom, edited by H.B. Gilbody, W.R. Newell, F.H. Read and A.C.H. Smith, Elsevier Science Publishers, Amsterdam. (1988).
66. L.A. Collins and B.I. Schneider, Ab Initio Methods for Electron-Molecule Collisions, *Electron-Molecule Scattering and Photoionization*, P.G. Burke and J.B. West, Eds., Plenum Publishing Co., 1988.
67. T.N. Rescigno, C.W. McCurdy and B.I. Schneider, Pseudospectral Techniques in Minimum Variance Calculations of Electron Scattering Cross Sections, *Phys. Rev.* **A38**, 5921 (1988).
68. T.N. Rescigno and B.I. Schneider, Vibration Effects in the b³Σ_u⁺ Excitation of H₂ by Electrons, *J. Phys. B.* **21**, L691 (1988).
69. B.I. Schneider and L.A. Collins, An Iteration-Variation Method for the Solution of Large Linear Systems, *Comp. Phys. Comm.*, **53**, 381 (1989).

70. B.I. Schneider and L.A. Collins, The Linear Algebraic Method for Electron Scattering, *Computer Physics Reports*, **10**, 49 (1989).
71. T.N. Rescigno, C.W. McCurdy and B.I. Schneider, Low Energy Scattering From Formaldehyde: A Complex Kohn Calculation, *Phys. Rev. Lett.* **63**, 248 (1989).
72. B.I. Schneider, T.N. Rescigno, C.W. McCurdy and B.H. Lengsfeld, III, Ab Initio Methods For The Treatment Of Electron Polyatomic Collisions, *Proceedings Of The ICPEAC Electron Molecule Satellite Conference*, New Haven, Conn., 1989, AIP Press, 1990.
73. M. Kushner, D. Hanson and B.I. Schneider, Reassessment of the Rate Constant for Electron Collision Quenching of Kr₂F(B), *Appl. Phys. Lett.* **55** (24), 2482 (1990)
74. B.I. Schneider, T. N. Rescigno and C.W. McCurdy, Vibrational Excitation of H₂CO: A Complex Kohn Calculation, *Phys. Rev.*, **A42**, 3132 (1990).
75. D.L. Lynch and B.I. Schneider, Generalization of the Linear Algebraic Method to 3-Dimensions, *Phys. Rev.* **A43** , 172 (1991).
76. B.I. Schneider, T.N. Rescigno, B.H. Lengsfeld and C.W. McCurdy, Accurate Ab Initio Treatment of Low Energy Electron Collisions With Ethylene, *Phys. Rev. Lett.* **66** , 2728 (1991).
77. T. N. Rescigno and B. I. Schneider, Electron Impact Excitation of the T and V States of Ethylene, *Phys. Rev.* **A45**, 2894 (1992).
78. D. L. Lynch and B. I. Schneider, Molecular Photoionization Using The Complex Kohn Method, *Phys. Rev.* **A45** , 4494 (1992).
79. L. A. Collins, B. I. Schneider and C. J. Noble, Electron Scattering from H₂⁺ : Resonances in Π Symmetry, *Phys. Rev.* **A45** , 4610 (1992)
80. K. Bhatia, B. I. Schneider and A. Temkin, Ab-Initio Method for Calculating Total Cross Sections, *Phys. Rev. Lett.* **70**, 1923 (1993)
81. B. I. Schneider, The Role of Theory in the Evaluation and Interpretation of Cross Section Data, *Advances in Atomic and Molecular Physics*, **33**, 1994, Academic Press
82. B. I. Schneider, An R-Matrix Approach to Electron-Molecule Collisions, *Computational Methods for Electron-Molecule Collisions*, p213, edited by Winifred M. Huo and Franco A. Gianturco, Plenum Press, New York, 1995.
83. L. A. Collins and B I. Schneider, The Linear Algebraic Method for Electron-Molecule Collisions, *Computational Methods for Electron-Molecule Collisions* p45, edited by Winifred M. Huo and Franco A. Gianturco, Plenum Press, New York, 1995
84. L. A. Collins, B. I. Schneider, D. L. Lynch and C. J. Noble, Electron Scattering from H₂⁺ : Resonances in the Σ and Π Symmetries. *Phys. Rev.* **A52**, 1310 (1995)
85. B. I. Schneider, Accurate Basis Sets for the Calculation of Bound and Continuum Wavefunctions of the Schrödinger Equation, *Phys. Rev.* **A55** , 3417 (1997).
86. B. I. Schneider and D. L. Feder, Numerical Approach to the Ground and Excited States of a Bose-Einstein Gas Confined in a Completely Anisotropic Trap, *Phys. Rev.* **A59** 2232 (1999)
87. D. L. Feder, C. W. Clark and B. I. Schneider, Vortex Stability of Interacting Bose-Einstein Condensates Confined in Anisotropic Harmonic Traps, *Phys. Rev. Lett.* **82**, 4956 (1999)
88. D. L. Feder, C. W. Clark and B. I. Schneider , Nucleation of Vortex Arrays in Rotating Anisotropic Bose-Einstein Condensates, *Phys. Rev.* **A61**, 011601 (2000)
89. J. Denschlag, J. E. Simarsian, D. L. Feder, C. W. Clark, L. A. Collins, J. Cubizolles, L. Deng, E. W. Hagley, K. Helmerson, W. P. Reinhardt, S. L. Rolston, B. I. Schneider and W. D. Phillips, Generating Solitons by Phase Engineering of a Bose-Einstein Condensate, *Science*, **287**, 97 (2000)
90. T. Bergeman, D. L. Feder, N. L. Balazs and B. I. Schneider, Bose Condensates in a Harmonic Trap Near the Critical Temperature, *Phys. Rev.* **A61**, 063605 (2000)

91. D.L. Feder, M.S. Pindzola, L.A. Collins, B.I. Schneider, C.W. Clark, Dark Soliton States of Bose-Einstein Condensates in Anisotropic Traps, *Phys. Rev.* **A62**, 052606 (2000)
92. B. I. Schneider and N. Nygaard, Orthogonal Polynomials, Gauss Quadratures and the Discrete Variable Representation, *J. Phys. Chem.* **A106(45)**, 10773, 2002
93. B. I. Schneider, L. A. Collins, and D. L. Feder, Computational Methods for the Solution of the Time-Dependent Schrödinger Equation, Proceedings of the International Workshop, From the Atomic to the Nanoscale, Editors C. Whelan and J. H. McGuire, Old Dominion University Press, December, 2002
94. L. A. Collins, S. Mazevet, J. D. Kress, B. I. Schneider, and D. L. Feder, Time-Dependent Simulations of Large-Scale Quantum Dynamics, Invited Paper, Proceedings of the XXIII ICPEAC, R. Schuch, H. Cederquist, M. Larsson and E. Lindroth (Eds.), American Institute of Physics (2004).
95. N. Nygaard, G. M. Brunn, B. I. Schneider, C. W. Clark and D. L. Feder, Vortex Line in a Neutral Finite Temperature Superfluid Fermi Gas, *Phys. Rev.* **A69**, 053622 (2004)
96. B. I. Schneider and N. Nygaard, Discrete Variable Representation for Singular Hamiltonians, *Phys. Rev. E* **70**, 056706 (2004)
97. B. I. Schneider and L. A. Collins, The Discrete Variable Method for the Time-Dependent Schrödinger Equation, *J. Non-Cryst. Solids*, **351**, 1351 (2005)
98. B. I. Schneider, L. A. Collins and S. X. Hu, Parallel Solver for the Time-Dependent Linear and Non-linear Schrödinger Equation, *Phys. Rev E* **73**, 036708 (2006) (Selected by editors of Virtual Journal of Ultrafast Science as an important contribution to the field)
99. N. Nygaard, B. I. Schneider and P. S. Julienne, Two Channel R-Matrix Analysis of Magnetic Field Induced Feshbach Resonances, *Phys. Rev* **A74**, 042705 (2006)
100. B. I. Schneider, Electron-Molecule Collisions: Quantitative Approaches and the Legacy of Aaron Temkin,, NASA GSFC Science Symposium on Atomic and Molecular Physics, NASA/CP-2006-214146, A. Bhatia, Editor, 2007
101. X. Guan, K. Bartschat, B. I. Schneider, O. Zatsarinny, J. Feist and C. J. Noble, A General Approach to Few-Cycle Intense Laser Interactions with Complex Atoms, *Phys. Rev* **A76**, 053411 (2007)
102. T. Simula, N. Nygaard, B. I. Schneider, L. A. Collins, S. X. Hu and K. Molmer, Angular Momentum Exchange Between Coherent Light and Matter Fields, *Phys. Rev.* **A77**, 015401 (2008)
103. X. Guan, K. Bartschat, B. I. Schneider, Dynamics of Two-photon Double Ionization of Helium in Short Intense XUV Laser Pulses, *Phys. Rev* **A77**, 043421 (2008)
104. J. Feist, S. Nagele, R. Pazourek, E. Persson, B. I. Schneider, L. A. Collins, and J. Burgdörfer, Non-Sequential Two-Photon Double Ionization of Helium, *Phys. Rev* **A77**, 043420 (2008)
105. X. Guan, C. J. Noble, O. Zatsarinny, K. Bartschat and B. I. Schneider, Time-Dependent R-Matrix Calculations for Multiphoton Ionization of Argon Atoms in Strong Laser Fields, *Phys. Rev.* **A78**, 053402 (2008)
106. J. Feist, S. Nagele, R. Pazourek, E. Persson, B. I. Schneider, L. A. Collins, and J. Burgdörfer, Probing Electron Correlation via Attosecond XUV Pulses in the Two-Photon Double Ionization of Helium, *Phys. Rev Lett.* **103**, 063002 (2009)
107. X. Guan, C. J. Noble, O. Zatsarinny, K. Bartschat and B. I. Schneider, ALTDSE: An Arnoldi-Lanczos Program to Solve the Time-Dependent Schroedinger Equation, *Computer Physics Communications*, **180**, 2401 (2009)
108. X. Guan, O. Zatsarinny, C. J. Noble, K. Bartschat and B. I. Schneider, Time-Dependent B-Spline, R-Matrix Approach to Double Ionization of Atoms by XUV Pulses, *J. Phys. B.* **192**, 032027 (2009)
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115. X. Guan, K. Bartschat and B. I. Schneider, Breakup of the Aligned H₂ Molecule by XUV Laser Pulses: A Time-Dependent Treatment in Prolate Spheroidal Coordinates, *Phys. Rev.* **A83**, 043403 (2011)
116. R. Pazourek, J. Feist, S. Nagele, E. Persson, B. I. Schneider, L. A. Collins and J. Burgdörfer, Universal Features in Sequential and Nonsequential Two-Photon Double Ionization of Helium, *Phys. Rev. A.* **83**, 053418 (2011)
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118. X. Guan, K. Bartschat and B. I. Schneider, Alignment Effect in Two-Photon Double Ionization of H₂ in Femtosecond XUV Laser Pulses, *Phys. Rev.* **A84**, 033420 (2011)
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122. X. Guan, K. Bartschat, B. I. Schneider, Breakup of the Aligned H₂ Molecule by XUV Laser Pulses: A Time-Dependent Treatment in Prolate Spheroidal Coordinates. *Physical Review A.* **83**, 043404 (2011)
123. X. Guan, E. Secor, K. Bartschat, B. I. Schneider, Double-slit Interference Effect in electron Emission from H₂⁺ Exposed to X-Ray Radiation. *Physical Review A.* **85**, 043419 (2012)
124. X. Guan, K. Bartschat and B. I. Schneider, Benchmark Calculations for Multi-Photon Ionization of the Hydrogen Molecule and the Hydrogen Molecular Ion by Short-Pulse Intense Laser Radiation, XSEDE '12 Proceedings of the 1st Conference of the Extreme Science and Engineering Discovery Environment: Bridging from the eXtreme to the campus and beyond, Article No. 17, ACM New York, NY, USA (2012)
125. B.I. Schneider, K. Bartschat, X. Guan, D. Feder, and L. A. Collins, Time-Dependent Computational Methods for Matter Under Extreme Conditions, submitted to *Advances in Chemical Physics* (2013).
126. T. R. Furlani, B. I. Schneider, M. D. Jones, J. Towns, D. L. Hart, S. M. Gallo, R. L. DeLeon, C-Da. Lu, A. Ghadersohi, R. J. Gentner, A. K. Patra, G. von Laszewski, F. Wang, J. T. Palmer, N. Simakov, Using XDMoD to Facilitate XSEDE Operations, Planning and Analysis, Presented, XSEDE-13, San Diego, California, July 2013
127. X Guan, K Bartschat, B. I. Schneider, L Koesterke, Resonance Effects in Two-Photon Double Ionization of H₂ by Femtosecond XUV Laser Pulses, *Physical Review A.* **88**, 043402 (2013)

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129. J. Feist, O. Zatsarinny, S. Nagele, R. Pazourek, J. Burgdörfer, X. Guan, K. Bartschat, and B. I. Schneider, Time delays for attosecond streaking in photoionization of neon, *Physical Review A* **89**, 033417 (2014)

INVITED TALKS

1. Electron Collisions Workshop, Belfast, Northern Ireland, 1976
2. International Symposium on the Quantum Theory of Atoms, Molecules, and Solids, Sanibel Island, Florida, January 1977.
3. X International Conference on the Physics of Electron and Atomic Collisions, Paris, France, 1977.
4. Five Problems in Electron-Molecule Collisions, Orsay, France, 1977.
5. Electron Molecule Collision Workshop and Asymptotic Methods in Electron Atom/Molecule Scattering, Daresbury Laboratory, UK, 1979.
6. University of Bari, Italy, 1979.
7. Electron Atom/Molecule Workshop, University of Bielefeld, West Germany, 1980.
8. Few-Body Problems in Physics, Gordon Conference, 1981.
9. DEAP, Boulder, Colorado, May 1983.
10. Electron-Molecule Processes, Rome, Italy, 1983.
11. SERC Workshop on Electron Scattering, University College , London, December 1983.
12. University of Paris South, Orsay, France, 1983 (two talks).
13. American Chemical Society Symposium on Resonances in Collision Processes, St. Louis, 1984.
14. Department of Physics, Louisiana State University, 1984.
15. Chairman, Application of Supercomputers in Atomic and Molecular Physics, DEAP Workshop, Norman, Oklahoma, May 1985
16. LURE, University of Paris South, Orsay, France, September 1986.
17. Physics Dept., University of Kaiserslautern, West Germany, October 1986.
18. Dept. of Physics, University of Oklahoma, November 1986.
19. XV ICPEAC, Brighton, England, 1987.
20. Physics Department, University of Heidelberg, 1988.
21. Physics Department University of Freiburg, 1988.
22. Physics Department University of Braunschweig, 1988.
23. Physics Department, University of Kaiserslautern, 1988.
24. Theoretical Chemistry Conference, Waldfischback, 1988.
25. University of Minnesota Supercomputer Workshop on Practical Iterative Methods for Large Linear Systems, October 1988.
26. Dept. of Physics, University of New Mexico, January 1989.
27. Electron Molecule Satellite Conference, New Haven, Conn., 1989.
28. NASA-Goddard Space Flight Center, December 1989.
29. NIST, February 1990.
30. Dept. of Physics, University of Maryland, April 1990.
31. Gaseous Electronics Conference, October 1991.

32. Dept. of Physics, Michigan State University, April, 1992
33. Electron-Molecule Workshop, ITAMP, March, 1993
34. Dept. of Physics, University of Virginia, April, 1993
35. Dept. of Physics, University of Central Florida, March 1994
36. DAMOP Washington, April, 1994
37. Dept. of Physics, University of Missouri/Rolla, October, 1994
38. Dept. of Chemistry, University of Southern California, October, 1994
39. Department of Physics, Texas A&M University, November, 1994
40. International Conference on the Application of Accelerators in Research and Industry, Denton, Texas, November, 1994
41. Dept. of Physics, Florida A&M University, November, 1994
42. Dept. of Physics and Astronomy, University of Oklahoma, December, 1994
43. Dept. of Physics, Boston College, March, 1995
44. Dept. of Physics, The University of Wisconsin, April, 1995
45. Texas Section of APS, October, 1995
46. Dept. of Physics, University of Nevada Reno, December, 1996
47. Dept. of Applied Physics. Princeton University, February, 1997
48. Queens University, Belfast. Festschrift for Professor P. G. Burke, October 1999
49. ITAMP Workshop on Computational Methods in Atomic and Molecular Physics, May, 2000
50. Physics Department, The University of Florida, April, 2001
51. Physics Department, Old Dominion University, April, 2002
52. ITAMP Workshop on Time-Dependent Methods in Quantum Mechanics, Harvard/ITAMP, May, 2002
53. Physics Department, Boston College, May, 2002
54. Old Dominion University, from the Atomic to the Nanoscale, December, 2002
55. University of Arizona, Weinberg Symposium, Oct. 2003
56. School of Computational Science, George Mason University, Feb. 2004
57. Physics Department, Georgia Tech, November, 2004
58. ITAMP Workshop on Attosecond Science, Harvard/ITAMP, April, 2005
59. NASA-Goddard Workshop in Atomic Collisions, Greenbelt MD, November, 2006
60. AURORA Supercomputing Conference, University of Vienna, June 18, 2007
61. Technical University of Vienna, June 29, 2007
62. National Institute for Computational Science, ORNL, June 2009
63. Plenary Speaker, TeraGrid-DEISA Summer School on Computational Science, Catania, Sicily, October 2010
64. George Mason School of Computational Science, September, 2010
65. Pacificchem, Honolulu, Hawaii, December, 2010
66. Institute for Physical Science and Technology, University of Maryland, February 2011
67. Keynote Speaker, Oklahoma Supercomputing Symposium, October, 2011
68. Keynote Speaker, UK Supercomputing Symposium, November, 2011

GRANTS

- NATO Grant to study Electron Molecule Collisions with L.A. Collins (Los Alamos) and Cliff Noble (Daresbury Laboratory, UK).
- IGPP Grant with N.T. Padial and J. Bellum, both at UNM Institute for Modern Optics for Photoionization and Photodissociation of Simple Molecular Species.
- Co-Principal Investigator on IGPP Grant to study Electronically Inelastic Scattering in Molecules of Atmospheric Interest.
- NATO Grant to study Vibrational Excitation and Dissociative Attachment in Diatomic Molecules with M. Le Dourneuf of Observatoire de Meudon, Paris, France

REVIEWER

- Physical Review
- Reviews of Modern Physics
- National Science Foundation (National and International)
- Physical Review Letters
- Journal of Chemical Physics
- Chemical Physics Letters
- Journal of Physics B
- Europhysics Letters
- Department of Energy
- EPSRC UK
- Journal of Computational Physics

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