

QTP Members

Faculty

Rodney J. Bartlett

Graduate Research Professor
Chemistry and Physics

Hai-Ping Cheng

Associate Professor
Physics Department

Erik Deumens

Scientist, Chemistry and Physics
QTP Computing Director

Frank E. Harris

Resident Adjunct Professor
Chemistry Department

Jeffrey L. Krause

Associate Professor
Chemistry Department

David A. Micha

Professor
Chemistry and Physics

Hendrik J. Monkhorst

Professor
Physics and Chemistry

N. Yngve Öhrn

Professor
Chemistry and Physics

Adrian E. Roitberg

Associate Scientist
Chemistry

John R. Sabin

Professor of Physics and Chemistry
D.I.R.T., CLAS

Samuel B. Trickey

Professor of Physics and Chemistry
Director, QTP

Adjunct Faculty

Jiri Cizek

University of Waterloo
Canada

Janet Del Bene

Youngstown State University
Ohio

Jan Linderberg

Åarhus University
Denmark

William H. Miller

University of California
Berkeley

Jens Oddershede

Odense University
Denmark

Neil S. Ostlund

Hypercube
Florida

Josef Paldus

University of Waterloo
Canada

QTP Members

Research Professor

Helena Hagelin
Chemistry Professor

Assistant Scientist

Ajith Perera
Chemistry (Bartlett)

Visiting Assistants

Norbert Flocke
Chemistry (Bartlett)

Piotr Rozyczko
Chemistry (Bartlett)

Postdoctoral Associates

Afaf Al Derzi
Chemistry (Bartlett)

John Ashley Alford III
Physics (Trickey)

Marshall Cory
Chemistry (Bartlett)

Stefan Fau
Chemistry (Bartlett)

Osamu Hino
Chemistry (Bartlett)

Andrew Kolchin
Physics (Cheng)

Victor Lotrich
Chemistry (Bartlett)

Monika Musial
Chemistry (Bartlett)

Rafal Podeszwa
Chemistry (Bartlett)

Keith Runge
Physics (Bartlett)

Remigio Trujillo
Physics (Sabin)

Graduate Students

Ariana Beste
Chemistry (Bartlett)

Ozlem Demir
Chemistry (Roitberg)

Maohua Du
Physics (Cheng)

Virgilio Fermo
Chemistry (Öhrn)

Thomas Henderson
Physics (Bartlett)

Paulo Herrera
Chemical Engineering (Micha)

Onder Kabadayi
Physics (Sabin)

Ben Killian
Chemistry (Öhrn)

Cem Kirman
Physics (Cheng)

Andrew Leathers
Chemistry (Micha)

Corneliu Manescu
Physics (Krause)

David Masiello
Chemistry (Öhrn)

Joshua McClellan
Chemistry (Bartlett)

Wilfredo Ortiz
Chemistry (Krause)

Alexander Pacheco
Chemistry (Micha)

Julio Palma
Chemistry (Roitberg)

Andres Reyes
Chemistry (Micha)

Alberto Santana
Chemistry (Micha)

Igor Schweigert
Chemistry (Bartlett)

Kevin Shuford
Chemistry (Krause)

Guangyu Sun
Physics (Trickey)

DeCarlos Taylor
Chemistry (Zerner/Bartlett)

Brian Thorndyke
Physics (Micha)

LinLin Wang
Physics (Cheng)

Hui Xiong
Physics (Roitberg)

Anthony Yau
Chemistry (Bartlett)

Dominika Zgid
Chemistry (Bartlett)

Chun Zhang
Physics (Cheng)

Wuming Zhu
Physics (Trickey)

Undergraduate Students

Robert Abel
Chemistry (Roitberg)

Ryan Chancey
Chemistry (Harris)

David Elm
Physics (Summer REU)

Nicholas Finck
Chemistry (Summer REU)

Luis Galiano
Chemistry (Summer KDI)

Anthony Hernandez
Chemistry (Micha)

Tom Hughes
Chemistry (Summer KDI)

Andrew Taube
Chemistry (Summer REU)

Sebastien Villaume
Chemistry (Summer REU)

Research Affiliates

Mark Ponton
CHSSI (Bartlett)

Anthony Yau
CHSSI (Bartlett)

Staff

Coralu Clements
Senior Word Processing
Operator

Antoinette Knight
Program Assistant (Bartlett)

Judy Parker
Office Manager

Arlene Roriguez
Senior Secretary

Adam Webb
Program Assistant (Bartlett)

Student Office Assistants

Sue Ellen Arnett
General Office &
Photographer

Rozanne Duchatellier
Web Pages

Lonnie Houck
Courier and
General Office

Ashley Sopotnick
General Office &
Photographer

Tiffany Wills
Fiscal Assistant

Ph.D.'s Granted

Andres Reyes

WITH PROFESSOR DAVID A. MICHA

Alberto Santana

with Professor David A. Micha

Kevin Shuford

with Associate Professor Jeffrey L. Krause

University Scholar Awards

Robert Abel

Roitberg Research Group

Ryan Chancey

Harris Research Group

Invited lectures

Rodney J. Bartlett

Advances in Electronic Structure Theory: Current Trends and Future Prospects, ICTCP-IV, Marly-le-Roi, France, July 2002.

Predictive Theory from Molecules to Materials, Science at the Edge, Michigan State University, September 2002.

Large Scale Dynamics with Quantum Mechanical Forces, Symposium and Summer School on Nano and Giga Challenges in Microelectronics Research and Opportunities, Moscow, Russia, September 2002.

Scalable Software for Computational Chemistry, University of Kentucky, Lexington, KY, October 2002.

Ab initio Predictions of PES for Chemical Reactions, MURI Kick-off Meeting, Aberdeen, MD, October 2002.

From Wave Function Theory to Density-Functional Theory and Back, New Orleans ACS National Meeting, March 2003

Frontiers in Theoretical Chemistry, A Symposium in honor of Prof. Rudolph A. Marcus, Los Angeles, CA, April 2003.

Predictive Methods from Molecules to Materials, National University of Ireland at Galway, Galway, Ireland, June 2003.

Hai-Ping Cheng

Understanding Hydrolytic Weakening at the Microscopic Level, Yangtze Conference, Yangtze River Boat, China, October 2002.

Multiscale Simulation of Water-Silica Interaction, Pan American Workshop, Cuernavaca, Mexico, Feb 2003.

Energetics and Electronic Structure of C_{60} on Surfaces and in Nanotubes, Mississippi State University, Mississippi State, MI, April 2003.

From surface to Cluster: A Computer Simulation of H_2O -Silica Interaction, University of Washington, Seattle, WA, May 2003.

Multi-Scale Quantum Simulation of Hydrolytic Weakening, seminar at Pacific Northwest National Laboratory, Richland, WA, May, 2003.

Erik Deumens

Annual Introduction to and Overview of the Capabilities and use of the John C. Slater Computing and Visualization Laboratory, University of Florida, QTP, September 18, 2002.

Problems in Quantum Mechanics, University of Florida, QTP, January 29, 2003.

Frank E. Harris

Fourier-Space Approach to Correlation in Polymers, University of Namur, Belgium, January 21, 2003.

Cumulant Approximations to Reduced Density Matrices, American Physical Society, Austin, TX, March 6, 2003.

Exponential Variational Expansions in Relative Coordinates, Queen's University, Kingston, Ontario, April 4, 2003.

Fourier-Representation Methods in Electronic-Structure Studies of Periodic Systems, CECAM, Lyon, France, May 15, 2003.

Treatment of Four-Body Problems using Relative Coordinates, University of Strasbourg, France, May 19, 2003.

Jeffrey L. Krause

Quantum Control in the Strong Response Regime, Department of Chemistry, Technical University of Denmark, Kongens Lyngby, Denmark, November 5, 2002.

Quantum Control in the Strong Response Regime, Department of Chemistry, University of Aarhus, Aarhus, Denmark, December 10, 2002.

Quantum Control in the Strong Response Regime, Instituto de Matemáticas y Física Fundamental, Consejo Superior de Investigaciones Científicas, Madrid, Spain, January 17, 2003.

Quantum Control in the Strong Response Regime, Department of Chemistry, University of Southern Denmark, Odense, Denmark, January 29, 2003.

Energy Transfer in Complex Systems, Annual March Meeting of the American Physical Society, Austin, Texas, March 2–7, 2003.

Quantum Control in the Strong Response Regime, VI Convegno on Complex Systems: Structure, Properties, Reactivity and Dynamics, Bologna, Italy, June 10–13, 2003.

David A. Micha

Dissipative Quantum Molecular Dynamics at Surfaces and in Clusters, Univ. of Florida QTP, Gainesville, FL., October 30, 2002.

Dissipative Dynamics of Femtosecond Desorption: CO/Cu(001), ACS South East Regional Meeting, S. Carolina, November 13–16, 2002.

Dissipative Quantum Dynamics at Surfaces and in Clusters, Pan-American Workshop, Cuernavaca, Mexico, Feb. 17–19, 2003.

Time Propagation of the Density Matrix for Dissipative Dynamics: Photodesorption by Femtosecond Pulses, American Chemical Society National Meeting, New Orleans, LA., March 23-27, 2003.

Hendrik J. Monkhorst

On Sustaining the p-11B Nuclear Resonance in a FRC Plasma, TriAlpha Energy, Inc. site, Lake Forest, CA (near Irvine, UC leased), November 22, 2002.

Celebrating More Than 2000 Citations of "Special Points for Brillouin Zone Integrations", Phys. Rev. B13, 5188 (1976) Very Special QTP Seminar, March 19, 2003.

In Support of Implementing the GW Method for Extended, Periodic Systems, CECAM Workshop, ENS, Lyon, France, May 16, 2003.

N. Yngve Öhrn

Electron Nuclear Dynamics, IVth International Congress of Theoretical Chemical Physics, Marly-le-Roi, Paris, France, July 9–16, 2002.

Proton Collisions with Organic Molecules at WATOC 2002, Lugano, Switzerland August 4–10, 2002.

Direct Nonadiabatic Molecular Reaction Dynamics, Institute of Quantum Chemistry, Uppsala University, Sweden, November 4 and 6, 2002.

Direct Nonadiabatic Molecular Reaction Dynamics, SERMACS 02 in Charleston, SC November 14–15, 2002.

Recent Results with Electron Nuclear Dynamics Theory, Department of Chemistry, Aarhus University, Denmark, May 8, 2003.

Direct, Nonadiabatic, Molecular Collision Theory, Werner Brandt Workshop, Playa del Carmen, Mexico, June 5, 2003.

Adrian E. Roitberg

Peptide and Protein Folding and Structure Prediction, University of Maryland Baltimore County, Baltimore, Maryland, September 2002.

Peptide and Protein Folding and Structure Prediction, Texas Tech. University, Lubbock, Texas, October 2002.

Protein Folding and Structure Prediction: Are we there yet?, Emory University, Atlanta, Georgia, March 2003.

John R. Sabin

Calculation of Molecular Stopping Cross Sections, International Conference on the Application of Accelerators in Research & Industry, Denton, Texas, November 12-16, 2002.

Low Energy Stopping Properties of Molecules, 2003 Pan-American Workshop on Molecular and Materials Sciences, Cuernavaca, Mexico, February 12-17, 2003.

Swift Ion-Molecule Collisions: Energy Transfer, 23rd Werner Brandt Workshop, Playa del Carmen, Mexico, June 3-6, 2003.

Samuel B. Trickey

Multi-scale, Multi-pass Simulations from Molecules to Materials, NSF DMR Computational Materials Theory Review meeting, University of Illinois Urbana-Champaign, June 19, 2002.

Method Development for Predictive Simulation of Chemo-Mechanical Processes in Materials, Sixth Pan American Workshop on Molecular and Materials Sciences, Cuernavaca México, February 17, 2003.

State of the Art for First Principles Calculation of Electronic Structure of Periodic Systems - Observations and Recommendations, CECAM Workshop on Rigorous *Ab Initio* Studies of Periodic Systems: Approaches to Electron Correlation, Lyon France, 14-16 May 2003.

Classical Potentials for Multi-scale Simulation of Fracture in Silica, Institut für Physikalische und Theoretische Chemie, Technische Universität München, Germany, 20 May 2003.



Erik Deumens & Hai-Ping Cheng. Erik, as Acting Director, was reading a congratulatory message from Jeff Krause at the going away party for Kevin Shuford, Jeff's first Ph.D. graduate.

Publications

RODNEY J. BARTLETT

S. Ivanov, S. Hirata and R. J. Bartlett, *Finite-Basis-Set Optimized Effective Potential Exchange-Only Method*, J. Chem. Phys. **116**, 1269-1276 (2002).

Szczepanski, J. Banisaukas, M. Vala, S. Hirata, R.J. Bartlett, and M. Head Gordon, *Vibrational and Electronic Spectroscopy of the Fluorene Cation*, J. Phys. Chem. A **106**, 63-73 (2002).

I. Grabowski, S. Hirata, S. Ivanov and R.J. Bartlett, *Ab Initio Density Functional Theory: OEP-MBPT(2) – a New Orbital-Dependent Correlation Functional*, J. Chem. Phys. **116**, 4415-4425 (2002).

A.D. Yau, S.A. Perera, and R.J. Bartlett, *Vertical Ionization Potentials of Ethylene: the Right Answer for the Right Reason*, Mol. Phys. **100**, 835-842 (2002).

S. Hirata, S. Ivanov, I. Grabowski, and R.J. Bartlett, *Time-Dependent Density Functional Theory Employing Optimized Effective Potentials*, J. Chem. Phys. **116**, 6468-6481 (2002).

J. E. Del Bene, S. A. Perera and R. J. Bartlett, *One-Bond (${}^{1d}J_{(H-H)}$) and Three-Bond (${}^{2d}J_{(X-M)}$) Spin-Spin Coupling Constants across X-H...H-M dihydrogen Bonds*, J. Chem. Phys. A **106**, 931- (2002).

M. Musial, S. Kucharski and R. J. Bartlett, *Diagrammatic Structure of the General Coupled Cluster Equations*, Mol. Phys. **100**, 1867-1872 (2002).

A. Beste, K. Runge and R. J. Bartlett, *Ensuring n -Representability: Coleman's Algorithm*, Chem. Phys. Lett. **355**, 263-269 (2002).

J. E. Del Bene, R. J. Bartlett and J. Elguero, *Interpreting ${}^{2h}J_{N-F'}$, ${}^{2h}J_{N-F}$ and ${}^{2h}J_{N-F}$ in the Hydrogen-Bonded FH:Collidine Complex*, Mag. Reson. Chem. **40**, 767- (2002).

M. Musial, S. A. Kucharski and R. J. Bartlett, *Formulation and Implementation of the Full Coupled-Cluster Method through Pentuple Excitations*, J. Chem. Phys. **116**, 4382-4388 (2002).

A. Beste and R. J. Bartlett, *The Electronic Structure of SiO₃: A Problematic Example for Coupled Cluster Methods*, Chem Phys. Lett. **366**, 100-108 (2002).

S. Fau, K. Wilson and R. J. Bartlett, *How Stable is N₅⁺N₅⁻?* J. Phys. Chem. A, **106**, 4639-4644 (2002).

M. Musial, S. A. Kucharski and R. J. Bartlett, *Equation-of-Motion Coupled Cluster Method with Full Inclusion of the Connected Triple Excitations for Ionized States: IP-EOM-CCSDT*, J. Chem. Phys. **118**, 1128-1136 (2002).

R. J. Bartlett, *To Multireference or Not to Multireference: That is the Question?*, Int. J. Mol. Sci. **3**, 579-603 (2002).

N. Flocke and R. J. Bartlett, *Localized Correlation Treatment using Natural Bond Orbitals*, Chem. Phys. Lett. **367**, 80-89 (2003).

- J.E. Del Bene, S.A. Perera, *Does the Magnitude of NMR Coupling Constants Specify Bond Polarity?*, Sym. Ser. ACS. **827**, 150-164 (2002).
- J. E. Del Bene, S.A. Perera, R.J. Bartlett, *Two-Bond C-13-N-15 Spin-Spin Coupling Constants ($^hJ(C-N)$) Across C-H-N Hydrogen*, J. Chem. Phys. **107** (18), 3222-3227 (2003).
- J. E. Del Bene, S.A. Perera, R.J. Bartlett, *Two-Bond F-19-N-15 Spin-Spin Coupling Constants ($^hJ(F-N)$) Across F-H Center Dot N Hydrogen Bonds*, J. Chem Phys. **107** (17), 3121-3125 (2003).
- J.E. Del Bene, S.A. Perera, R.J. Bartlett, *Two Bond N-15-F-19 Spin-Spin Coupling Constants ($^hJ(N-F)$) Across N-H + Center Dot Center Dot F Hydrogen Bonds*, J. Chem Phys. **17**, 3126-3131 (2003).
- T. M. S. Hirata, R. J. Bartlett, *The Analytical Energy Gradient Scheme in the Gaussian Based Hartree-Fock and Density Functional Theory for Two-Dimensional Systems using the Fast Multipole Method*, J. Chem. Phys. **118** (13), 5776-5792, (2003).
- J.E. Del Bene, K. Runge, R.J. Bartlett, *A Quantum Chemical Mechanism for the Water-Initiated Decomposition of Silica*, Comp. Mater Sci. **27** (1-2), 204-211, (2003).
- C.E. Taylor, M.G. Cory, R.J. Bartlett, *The Transfer Hamiltonian: a Tool for Large Scale Simulations with Quantum Mechanical Forces*, Comp. Mater Sci. **27** (1-2): 204-211, (2003).
- N. Flocke, R.J. Bartlett, *Correlation Energy Estimates in Periodic Extended Systems using the Localized Natural Bond Orbital Coupled Cluster Approach*, J. Chem. Phys. **118** (12), 5326-5334, (2003).
- M. Musial, S.A. Kucharski, R.J. Bartlett, *Equation-of-Motion Coupled Cluster Method with Full Inclusion of the Connection Triple Excitations for Ionized States: IP-EOM-CCSDT*, J. Chem. Phys. **118** (3), 1128-1136, (2003).
- N. Focke, R. J. Bartlett, *Localized Correlation Treatment using Natural Bond Orbitals*, Chem. Phys. Lett. **367** (1-2), 80-89, (2003).
- S. Ivanov, S. Hirata, I. Grabowski, *Connections Between Second-Order Gorling-Levy and Many-Body Perturbation Approaches in Density Functional Theory*, J. Chem. Phys. **118** (2), 461-470, (2003).
- T. M. Henderson, K. Runge and R. J. Bartlett, *Excited States in Artificial Atoms via the Equation-of-Motion Coupled Cluster Theory*, Phys. Rev. B, **67**, 045320 (2003).
- S. Ivanov, S. Hirata, I. Grabowski, and R.J. Bartlett, *Connections Between Görling-Levy and Many-Body Perturbation Approaches in Density Functional Theory*, in press.
- M. Tobita, S. Hirato and R. J. Bartlett, *The Analytical Energy Gradient Scheme in the Gaussian Based Hartree-Fock and Density Functional Theory for Two-Dimensional Systems using Fast Multipole Method*, J. Chem. Phys., in press.
- J. E. Del Bene, S. A. Perera and R. J. Bartlett, *Two-Bond $^{13}C-^{15}N$ Spin-Spin Coupling Constants Across ($^hJ_{C-N}$) C-H-N Hydrogen Bonds*, J. Phys. Chem., in press.
- C.E. Taylor, M. Cory, W. Thiel and R.J. Bartlett, *The Transfer Hamiltonian: Parameterization of Semi-Empirical NDDO Hamiltonians using Ab initio Coupled Cluster Theory*, J. Comput. Material Sci., in press.
- N. Flocke and R. J. Bartlett, *Correlation Energy Estimates in Periodic Extended Systems using the Localized NBO Coupled Cluster Approach*, J. Chem. Phys., in press.

HAI-PING CHENG

J.G. Polihronov, R.E. Hummel, and H.-P. Cheng, *Optical Properties and Energetics of Silicon Ring-Shaped Clusters in Amorphous SiO₂*, J. Lumin. vol. **101**, No.1-2, 55-62 (2002).

H.-P. Cheng, R.N. Barnett, and U. Landman, *Structure, Collective Hydrogen Transfer and Formation of Si(OH)₄ in SiO₂-H₂O Clusters*, J. Chem. Phys. **116**, 9300 (2002).

M.-H. Du and H.-P. Cheng, *A Transparent Interface between Classical Molecular Dynamics and the First Principles Molecular Dynamics*, IJQC, Vol. **93**, 1 (2003).

M. Schmidt, Ph. Cahuzac, C. Brechignac and H.-P. Cheng, *Stability of Free and Oxidized Silver Clusters*, J. Chem. Phys. (in press) (2003).

M.-H. Du, L.-L. Wang, A. Kolchin, and H.-P. Cheng, *Water-Silica Interactions in Cluster*, (J. Euro. Phys. in press).

ERIK DEUMENS

R. Cabrera-Trujillo, Y. Öhrn, J. R. Sabin and E. Deumens, *Molecular Target and Projectile Angular Scattering Effects in Stopping Power and Charge Exchange at Low-to-Intermediate Projectile Energies*, Phys. Rev. A **65**, 24901 (2002).

R. Cabrera-Trujillo, Y. Öhrn, E. Deumens, and J. R. Sabin, *Trajectory and Molecular Binding Effects in Stopping Cross Section for Hydrogen Beams on H₂*, J. Chem. Phys. **116** (7), 2783–2793 (2002).

Mauricio Coutinho-Neto, Erik Deumens, and Y. Öhrn, *Abstraction and Exchange Mechanisms for the D₂+NH₃⁺ Reaction at Hyperthermal Collision Energies*, J. Chem. Phys. **116** (7), 2794–2802 (2002).

F. Hagelberg and E. Deumens, *Nonadiabatic Effects in the Pseudorotational Motion of Triatomic Molecules*, Phys. Rev. A **65**, 052505 (2002).

R. Cabrera-Trujillo, J. R. Sabin, Erik Deumens and Y. Öhrn, *Dynamics of Proton-Acetylene Collisions at 30 eV*, S. A. Malinovskaya, J. Chem. Phys. **117** (3), 1103–1108 (2002).

R. Cabrera-Trujillo, J. R. Sabin, E. Deumens, and Y. Öhrn, *Stopping Cross Sections for N⁴⁺H at Low Projectile Velocity*, Phys. Rev. A **66**, 022706 (2002).

D. Jacquemin, B. Champagne, J.M. André, E. Deumens, and Y. Öhrn, *Integral Algorithm and Density Matrix Integration Scheme for ab initio Band Structure Calculations on Polymeric Systems*, J. Comp. Chem. **23** (15), 1430–1444 (2002).

R. Cabrera-Trujillo, Y. Öhrn, E. Deumens, J. R. Sabin, B. G. Lindsay, *Theoretical and Experimental Studies of the H+ N₂ System: Differential Cross Sections for Direct and Charge-Transfer Scattering at keV Energies*, Phys. Rev. A **66**, 042712 (2002).

R. Cabrera-Trujillo, J. R. sabin, Y. Öhrn, E. Deumens, *Case for Negative Stopping Power*, Phys. Rev. A (2002) submitted.

FRANK E. HARRIS

F. E. Harris, Analytic Quadratic Integration Over the Two-Dimensional Brillouin Zone, *J. Physics: Condensed Matter* **14**, 621-630 (2002).

F. E. Harris, Comments on "Wald Summation Technique for One-Dimensional Charge Distributions," *Comput. Phys. Commun.* **146**, 271-273 (2002).

Q.-H. Tang, K. Runge, H.-P. Cheng, & F. E. Harris, *Orientation Dependence in C_{60} Surface-Impact Collisions*, *J. Phys. Chem A* **106**, 893-896 (2002).

J. Delhalle, J. G. Fripiat, & F. E. Harris, *Exchange Contributions in the Electronic Structure of Systems with 1D-Periodicity: Importance and Computation*, *Int. J. Quantum Chem.* **90**, 587-593 (2002).

F.E. Harris, *Cumulant-Based Approximations to Reduced Density Matrices*, *Int. J. Quantum Chem.* **90**, 105-113 (2002).

F. E. Harris, *Analytical Evaluation of Two-Center STO Electron Repulsion Integrals via Ellipsoidal Expansion*, *Int. J. Quantum Chem.* **88**, 701-734 (2002).

W. Gautschi, F. E. Harris & N. M. Temme, *Expansions of the Exponential Integral in Incomplete Gamma Functions*, *Appl. Math. Lett.* (in press).

J. Delhalle, J. G. Fripiat & F. E. Harris, *Virtues and Potentialities of the Fourier Transform Method for Electronic Structure Calculations of 1D Periodic Systems at the Hartree-Fock Level and Beyond*, *Int. J. Quantum Chem.* **90**, 1326-1333 (2002).

R. T. Chancey, L. Oddershede, F. E. Harris & J. R. Sabin, *Fragmentation of Fullerenes*, *Phys. Rev. A* **67**, 043203 (1-7) (2003).

F. E. Harris, *Comment on "Computation of Two-Center Coulomb Integrals over Slater-Type Orbitals Using Elliptical Coordinates"*, *Int. J. Quantum Chem.* **93**, 332-334 (2003).

JEFFREY L. KRAUSE

Kevin L. Shuford and Jeffrey L. Krause, *Control of Wave Packet Dynamics in Quantum Wells: Effects of Coulomb Interactions*, *Journal of Applied Physics* **91**, 6533-6538 (2002).

Kevin L. Shuford and Jeffrey L. Krause, *Controlling THz Emission from Quantum Wells*, *Journal of Physical Chemistry A* **106**, 10818-10824 (2002).

Maria Pilar de Lara-Castells and Jeffrey L. Krause, *Theoretical Study of the UV-Induced Desorption of Molecular Oxygen from the Reduced TiO_2 (110) Surface*, *Journal of Chemical Physics* **118**, 5098-5104 (2003).

Kevin L. Shuford and Jeffrey L. Krause, *Adiabatic passage in quantum wells via DC fields*, *Journal of Physics D: Applied Physics* **36**, 439-445 (2003).