Christine M. Isborn

Professor
Chemistry and Biochemistry
University of California, Merced
5200 Lake Road
Merced, CA 95343

email: cisborn@ucmerced.edu
office phone: 209-228-4693
http://faculty.ucmerced.edu/cisborn

Professional Experience

Chair of the UC Merced Chemistry and Biochemistry Graduate Program 7/20 –
Professor 7/23 –
Associate Professor 7/19 – 7/23
Assistant Professor 8/12 – 7/19
Chemistry and Biochemistry, University of California, Merced

Electronic excitation and dynamics, charge-transfer in complex environments, optical properties of chromophores in the condensed phase, linear and nonlinear spectroscopy

Post-doctoral Researcher 9/09 – 7/12
Chemistry Department, Stanford University
Postdoctoral Advisor: Todd Martínez

Implementation of CIS and TDDFT into existing GPU accelerated quantum chemistry code, interfacing QM and MM methods. Applications to studies of photophysics in fluorescent proteins, solvation

Education

Ph.D. Chemistry University of Washington 2009
Doctoral advisor: Xiaosong Li

Non-adiabatic dynamics, modeling molecular interactions with intense laser fields using Ehrenfest dynamics with time-dependent density functional theory (TDDFT), first principles electron dynamics, multi-electron excitations

M.S. Chemistry University of Washington 2005
Advisors: Weston Thatcher Borden, Bruce Robinson, Bart Kahr

Calculation of molecular optical properties such as hyperpolarizabilities and optical rotatory tensors, ab initio and multi-configurational calculations on open-shell organic molecules

B.S. Chemistry and Physics University of San Francisco 2001
summa cum laude

Honors and Awards

- UC Merced Senate Award for Distinguished Early Career Research 2018
- ACS Open Eye Outstanding Junior Faculty Award in Computational Chemistry 2016
- Hellman Faculty Fellow 2014
- NIH Ruth L. Kirschstein NRSA post-doctoral fellow 2010-2012

Research Support / Grants Received

Department of Defense, U.S. Air Force Office of Scientific Research 2022-2027
$7,500,000 *MURI: Polartion Chemistry* (Isborn is co-PI; $1,200,000 for UC Merced)

National Science Foundation (CTMC) 2020-2023
$435,000 *Improved Methods for Including Vibronic and Environmental Effects in Simulations of Optical Spectroscopy*

Department of Energy, Basic Energy Sciences (CTC) 2019-2022
$1,200,000 *Applying Deep Learning Methods to Develop New Models of Charge Transfer, Nonadiabatic Dynamics, and Nonlinear Spectroscopy in the Condensed Phase* (Isborn is PI; $804,584 for UC Merced)

Department of Energy, Basic Energy Sciences (CTC and CPIMS) 2018-2021
$1,580,000 *Improved Methods for Modeling Functional Transition Metal Compounds in Complex Environments: Ground States, Excited States, and Spectroscopies* (Isborn is co-PI with UC Merced faculty Hratchian, Pribram-Jones, Shi, and Strubbe)

National Science Foundation 2018-2023
$1,500,000 *Building Capacity: Improving the Undergraduate Chemistry Experience at HSIs by Bridging the GAP (through Green chemistry, Active-learning, and Peer-led experiences)*
(Isborn is co-PI with UC Merced faculty Menke, Hratchian, Leslie, and Stokes)

Silicon Mechanics 2016
High Performance Computing Cluster PI, for an HPC Cluster worth ~$100,000

Department of Energy, Basic Energy Sciences (CTC and CPIMS) 2015-2019
$1,289,956 *Development of Approaches to Model Excited State Charge and Energy Transfer in Solution* (Isborn is PI; $484,996 for UC Merced)

Department of Defense, U.S. Air Force Office of Scientific Research 2015-2019
$595,511 *Improved Prediction of the Optical Properties of Coupled Chromophores for Electro-Optics (research and educational components)*

American Chemical Society Petroleum Research Fund 2014-2016
$100,000 *Quantum Mechanical Calculations of Large-Scale Solvation*

Hellman Faculty Fellow 2014
$20,000 *Modeling Molecular Charge and Energy Transfer in Solution*

Teaching

- *Chem 10 – General Chemistry* 2019, 2020
- *Chem 130 – Computational Chemistry* 2016, 2018
- *Chem 10H – Honors General Chemistry* 2014
- *Chem 112 – Quantum Chemistry and Spectroscopy* 2012-19
- *Chem 212 – Graduate Quantum Chemistry* 2021

Synergistic Activities

- Co-organizer and lecturer for Time-Dependent Density Functional Theory Summer School at Telluride Science Research Center, 2017, Rutgers, Newark, 2019, TBD 2023
- Co-organizer for 2014, 2015, 2017 Telluride Science Research Center and 2019 Rutgers workshops on modeling electronic excited states
- Mentor for ACS Project SEED: a summer research internship program for economically disadvantaged high school students
- Mentor in UC Merced's Undergraduate Research and Mentoring Program in Computational Biology, UC Merced's NSF-funded REU in Applications in Modern Materials
- Trained in CIMER's "Facilitating Entering Research and Curriculum Development Institute", May 2021 and "Facilitating Entering Mentoring", January 2022
- American Chemical Society PHYS Theory Subdivision Vice-Chair (2021), Chair-Elect (2022), Chair (2023)
- UC Merced's representative on the Faculty Advisory Committee of the Presidential Postdoctoral Fellowship Program (2022-2025)

Publications (h-index on google scholar is 37 as of July 1, 2023)

73. Michael S. Chen, Yuezhi Mao, Andrew Snider, Prachi Gupta, Andrés Montoya-Castillo, . Zuehlsdorff, Christine M. Isborn, Thomas E. Markland. "Elucidating the Role of Hydrogen Bonding in the Optical Spectroscopy of the Solvated Green Fluorescent Protein Chromophore: Using Machine Learning to Establish the Importance of High-Level Electronic Structure." *J. Phys. Chem. Lett.* 14, 6610. 2023

72. Karnamohit Ranka, Christine M. Isborn. "Size-Dependent Errors in Real-Time Electron Density Propagation." *J. Chem. Phys*. 158, 174102. 2023

71. Bowen Han, Christine M. Isborn, Liang Shi. "Incorporating Polarization and Charge Transfer in a Point-Charge Model for Water using Machine Learning." *J. Phys. Chem. Lett*. 14, 3869. 2023

70. Chiao-Yu Cheng, Alyssa Brigeman, Ajay Khanna, Sapana Shedge, Christine M. Isborn, Joel Yuen-Zhou, Noel C. Giebink. "Molecular Polariton Electroabsorption." *Nature Communications* 13, 7937. 2022

69. Harish S. Bhat, Kevin Collins, Prachi Gupta, Christine M. Isborn. "Dynamic Learning of Correlation Potentials for a Time-Dependent Kohn-Sham System." *Proceedings of Machine Learning Research, Learning for Dynamics and Control Conference.* 168. 546-558. 2022

68. Ali Abou Taka, Shao-Yu Lu, Duncan Gowland, Tim J. Zuehlsdorff, Hector H. Corzo, Aurora Pribram-Jones, Liang Shi, Hrant P. Hratchian, Christine M. Isborn. "Comparison of Linear Response Theory, Projected Initial Maximum Overlap Method, and Molecular Dynamics Based Vibronic Spectra: The Case of Methylene Blue." *J. Chem. Theory Comp.* 18 3039-3051. 2022

67. Prachi Gupta, Harish S. Bhat, Karnamohit Ranka, Christine M. Isborn. "Statistical Learning for Predicting Density-Matrix Based Electron Dynamics." *Stat.* e439. 2022

66. Shao-Yu Lu, Tim J. Zuehlsdorff, Hanbo Hong, Vincent P. Aguirre, Christine M. Isborn, Liang Shi. "The Influence of Electronic Polarization on Nonlinear Optical Spectroscopy." *J. Phys. Chem. B* 125, 12214-12227. 2021

65. Angus J. Dunnett, Duncan Gowland, Christine M. Isborn, Alex W. Chin, Tim J. Zuehlsdorff. "Influence of Non-Adiabatic Effects on Linear Absorption Spectra in the Condensed Phase." *J. Chem. Phys.* 155, 144112. 2021

64. Sapana V. Shedge, Tim J. Zuehlsdorff, Ajay Khanna, Stacey Conley, Christine M. Isborn. "Vibronic and Environmental Effects in Simulations of Optical Spectroscopy." *J. Chem. Phys.* 154, 084116. 2021

63. Bowen Han, Christine M. Isborn, Liang Shi. "Determining Partial Atomic Charges for Liquid Water: Assessing Electronic Structure and Charge Models." *J. Chem. Theory Comp.* 17, 889-901. 2021

62. Tim J. Zuehlsdorff, Sapana V. Shedge, Shao-Yu Lu, Hanbo Hong, Vincent P. Aguirre, Liang Shi, Christine M. Isborn. "Vibronic and Environmental Effects in Simulations of Optical Spectroscopy." *Annual Review of Physical Chemistry* 72, 165-188. 2021

61. Stefan Seritan, Christoph Bannwarth, Bryan S. Fales, Edward G. Hohenstein, Christine M. Isborn, Sara I. L. Kokkila-Schumacher, Xin Li, Fang Liu, Nathan Luehr, James W. Snyder Jr., Chenchen Song Alexey V. Titov, Ivan S. Ufimtsev, Lee-Ping Wang, Todd J. Martinez. "TeraChem: A Graphical Processing Unit-Accelerated Electronic Structure Package for Large-Scale ab initio Molecular Dynamics." *Wiley Interdisciplinary Reviews: Computational Molecular Science, e1494*. 2021

60. Harish S. Bhat, Karnamohit Ranka, Christine M. Isborn. "Machine Learning a Molecular Hamiltonian for Predicting Electron Dynamics." *Int. J. Dynamics and Control*. 8, 1089-1101. 2020

59. Xiaosong Li, Niranjan Govind, Christine M. Isborn, Eugene A. DePrince, Kenneth Lopata. "Real-Time Time-Dependent Electronic Structure." *Chem. Rev*. 120, 9951-9993. 2020

58. Michael Chen, Tim J. Zuehlsdorff, Thomas Morawietz, Christine M. Isborn, Thomas E. Markland. "Exploiting Machine Learning to Efficiently Predict Multidimensional Optical Spectra in Complex Environments." *J. Phys. Chem. Lett.* 11, 7559-7568, 2020

57. Tim J. Zuehlsdorff, Hanbo Hong, Liang Shi, Christine M. Isborn. "Nonlinear Spectroscopy in the Condensed Phase: the Role of Duschinsky Rotations and Third Order Cumulant Contributions." *J. Chem. Phys.* 153, 044127. 2020

56. Christine M. Isborn. "The Link Between Electrolytes and Metals." Invited Perspective. *Science* 368, 1056-1057. 2020

55. Tim J. Zuehlsdorff, Hanbo Hong, Liang Shi, Christine M. Isborn. "Influence of Electronic Polarization on the Spectral Density." *J. Phys. Chem. B* 124, 531-543. 2020

54. Aleksey Kocherzhenko, Sapana V. Shedge, Pauline F. Germaux, Mohammed Heidarian, Christine M. Isborn. "Excitonic Hamiltonians for Calculating Optical Absorption Spectra and Optoelectronic Properties of Molecular Aggregates and Solids." *JoVE* 159, e60598. 1940-087X. 2020

53. Makenzie Provorse Long, Serra Alland, Madison Martin, Christine M. Isborn. "Molecular dynamics simulations of alkaline earth metal ions binding to DNA reveal ion size and hydration effects." *Phys. Chem. Chem. Phys.* 22, 5584-5596. 2020

52. Tim J. Zuehlsdorff, Andrés Montoya-Castillo, Joseph A. Napoli, Thomas E. Markland, Christine M. Isborn. "Optical Spectra in the Condensed Phase: Capturing Anharmonic and Vibronic Features using Dynamics and Static Approaches" *J. Chem. Phys.* 151, 074111. 2019

51. Sapana V. Shedge, Tim J. Zuehlsdorff, Michael J. Servis, Aurora E. Clark, Christine M. Isborn. "The Effect of Ions on the Optical Absorption Spectra of Aqueously Solvated Chromophores." *J. Phys. Chem. A* 123, 6175-6184, 2019

50. Aleksey A. Kocherzhenko, Sapana Shedge, Xochitl A. Sosa Vazquez, Jessica Maat, Jacob Wilmer, Andreas F. Tillack, Lewis E. Johnson, Christine M. Isborn. "Unraveling Excitonic Effects for the First

Hyperpolarizabilities of Chromophore Aggregates." *J. Phys. Chem. C* 123, 13818-13836. 2019. **Cover article**

49. Tim J. Zuehlsdorff, Christine M. Isborn. "Modeling Absorption Spectra of Molecules in Solution." Invited Perspective for *Int. J. Quantum Chem.* 119, e25719. 2019. **Cover article**

48. Tim J. Zuehlsdorff, Joseph A. Napoli, Joel M. Milanese, Thomas E. Markland, Christine M. Isborn. "Unraveling Electronic Absorption Spectra using Nuclear Quantum Effects: Photoactive Yellow Protein and Green Fluorescent Protein Chromophores in Water." *J. Chem. Phys.* 149, 024107. 2018

47. L. E. Johnson, D. L. Elder, A. A. Kocherzhenko, A. F. Tillack, C. M. Isborn, L. R. Dalton, B. H. Robinson. "Poling-induced birefringence in OEO materials under nanoscale confinement." *J. Lightwave Tech.* 36, 5036-5047. 2018

46. B. H. Robinson, L. E. Johnson, D. L. Elder, A. A. Kocherzhenko, C. M. Isborn, C. Haffner, W. Heni, C. Hoessbacher, Y. Fedoryshyn, Y. Salamin, B. Baeuerle, A. Josten, M. Ayata, U. Koch, J. Leuthold, L. R. Dalton. "Optimization of Plasmonic-Organic Hybrid Electro-Optics." *Proc. SPIE 10738, Organic Photonics and Electronics, Organic and Hybrid Sensors and Bioelectronics XI,* 107381A. 2018

45. Tim J. Zuehlsdorff, Christine M. Isborn. "Combining the Ensemble and Franck-Condon Approaches for Calculating Spectral Shapes of Molecules in Solution." *J. Chem. Phys.* 148, 024110. 2018. **Chosen as an Editor's Pick.**

44. Makenzie R. Provorse Long, Christine M. Isborn. "Combining Explicit Quantum Solvent with a Polarizable Continuum Model." *J. Phys. Chem. B* 121, 10105-10117. 2017

43. Aleksey A. Kocherzhenko, Xochitl A. Sosa Vazquez, Joel M. Milanese, Christine M. Isborn. "Absorption Spectra for Disordered Aggregates of Chromophores Using the Exciton Model." *J. Chem. Theory Comp.* 13, 3787-3801. 2017

42. Joel M. Milanese, Makenzie R. Provorse, Enrique Alameda Jr., Christine M. Isborn. "Convergence of Computed Aqueous Absorption Spectra with Explicit Quantum Mechanical Solvent." *J. Chem. Theory Comp.* 13, 2159-2171. 2017

41. Makenzie R. Provorse, Thomas Peev, Chou Xiong, Christine M. Isborn. "Convergence of Excitation Energies in Mixed Quantum and Classical Solvent: Comparison of Continuum and Point Charge Models." *J. Phys. Chem. B* 120, 12148-12159. 2016

40. Lu Wang, Christine M. Isborn, Thomas E. Markland. "Simulating Nuclear and Electronic Quantum Effects in Enzymes." *Methods in Enzymology*. 577, 389-418. 2016

39. Makenzie R. Provorse, Christine M. Isborn. "Electron Dynamics with Real-Time Time-Dependent Density Functional Theory." *Int. J. Quantum Chem*. 116, 739-749. 2016. DOI: 10.1002/qua/25096. 116, 739-749. 2016

38. Xochitl A. Sosa Vazquez, Christine M. Isborn. "Size-Dependent Error of the Density Functional Theory Ionization Potential in Vacuum and Solution." *J. Chem. Phys*. 143, 244105. 2015

37. Makenzie R. Provorse, Bradley F. Habenicht, Christine M. Isborn. "Peak-Shifting in Real-Time Time-Dependent Density-Functional Theory." *J. Chem. Theory Comp.* 11, 4791-4802. 2015

36. Sarah R. Whittleton, Xochitl A. Sosa Vazquez, Christine M. Isborn, Erin R. Johnson. "Density-functional Errors in Ionization Potential with Increasing System Size." *J. Chem. Phys*. 142, 1184106. 2015

35. Bradley F. Habenicht, Noriyuki Tani, Makenzie R. Provorse, Christine M. Isborn. "Two-Electron Rabi Oscillations in Real-Time Time-Dependent Density-Functional Theory." *J. Chem. Phys*. 141, 184112. 2014

34. Kerry Garrett, Xochitl Sosa Vazquez, Shawn B. Egri, Jacob Wilmer, Lewis E. Johnson, Bruce H. Robinson, Christine M. Isborn. "Optimum Exchange for Calculation of Excitation Energies and Hyperpolarizabilities of Organic Electro-Optic Chromophores." *J. Chem. Theory Comp.* 10, 3821-3831. 2014

33. Christine M. Isborn, Brendan D. Mar, Basile F. E. Curchod, Ivano Tavernelli, Todd J. Martinez. "The Charge Transfer Problem in Density Functional Theory Calculations of Aqueously Solvated Molecules." *J. Phys. Chem. B.* 117, 12189-12201, 2013

32. Christine M. Isborn, Chun Tang, Ashlie Martini, Erin R. Johnson, Alberto Otero-de-la-Roza, Vincent C. Tung. "Carbon Nanotube Chirality Determines Efficiency of Electron Transfer to Fullerene in All-Carbon Photovoltaics." *J. Phys. Chem. Lett.* 4, 2914-2918. 2013

31. Christine M. Isborn, Andreas W. Götz, Matthew A. Clark, Ross C. Walker, Todd J. Martinez. "Computing Electronic Absorption Spectra from MM and ab initio QM/MM Molecular Dynamics: Exploring Environmental Effects on the Absorption Spectrum of Photoactive Yellow Protein." *J. Chem. Theory Comp.* 8, 5092-5106. 2012

Published before starting as a faculty member at UC Merced:

30. Feizi Ding, Wenkel Liang, Craig Chapman, Christine M. Isborn, Xiaosong Li. "On the Gauge Invariance of Nonperturbative Electronic Dynamics using Time-Dependent Hartree-Fock and Time-Dependent Density Functional Theory." *J. Chem. Phys*. 135, 164101. 2011

29. Christine M. Isborn, Nathan Luehr, Ivan S. Ufimtsev, Todd J. Martinez. "Excited State Electronic Structure with CIS and TDA-TDDFT on Graphical Processing Units (GPUs)." *J. Chem. Theory Comput*. 7, 1814-1823. 2011

28. Sean A. Fischer, Christine M. Isborn, Oleg V. Prezhdo "Excited States and Optical Absorption of Small Semiconductor Clusters: Dopants, Defects, and Charging." *Chemical Science* 2, 400-406. 2011

27. Yonghong Bing, David Selassie, Christine M. Isborn, Werner Kaminsky, Bart Kahr. "Resolution and Racemization of an Unhindered Triarylmethyl Propeller in Sodium Chlorate Crystals Monitored by Its Circular Dichroism Tensor." *J. Am. Chem. Soc*. 132, 7454-7465. 2010

26. Wenkel Liang, Christine M. Isborn, Alex Lindsay, Xiaosong Li, Stanley M. Smith, Robert J. Levis. "Time-Dependent Density Functional Theory Calculations of Ehrenfest Dynamics of Laser Controlled Dissociation of NO+: Pulse Length and Sequential Multiple Single-Photon Processes." *J. Phys. Chem. A* 114, 6201-6206. 2010

25. Sean A. Fischer, Angeline B. Madrid, Christine M. Isborn, Oleg V. Prezhdo. "Multiple Exciton Generation in Small Si Clusters: A High-Level, Ab Initio Study." *J. Phys. Chem. Lett.* 1, 232-237. 2010

24. Wenkel Liang, Christine M. Isborn, Xiaosong Li. "Obtaining Doubly Excited States with Real-time Time-dependent Hartree-Fock and Density Functional Theory." *J. Chem. Phys*. 131. 204101. 2009

23. Christopher Moss, Christine M. Isborn, Xiaosong Li. "Ehrenfest Dynamics with Time-Dependent Density Functional Theory: Lifetime and Charge Neutralization Rates of an Excited State Lithium Atom Near an Aluminum Cluster Surface." *Phys. Rev. A* 80, 024503. 2009

22. Christine M. Isborn, Oleg V. Prezhdo. "Charging Quenches Multiple Exciton Generation in Semiconductor Nanocrystals." *J. Phys. Chem. C* 113, 12617-12621. 2009

21. Christine M. Isborn, Xiaosong Li. "Singlet-Triplet Transitions in Real-Time Time-Dependent Hartree-Fock/Density Functional Theory." *J. Chem. Theory Comput*. 5, 2415-2419. 2009

20. Ekaterina Badaeva, Christine M. Isborn, Yong Feng, Stefan Ochsenbein, Daniel Gamelin, Xiaosong Li. "Theoretical Characterization of Electronic Transitions in Co^{2+} and Mn^{2+} Doped ZnO Nanocrystals." *J. Phys. Chem. C* 113, 8710-8717. 2009

19. Wenkel Liang, Christine M. Isborn, Xiaosong Li. "Laser Controlled Dissociation of $C_2H_2^{2+}$: Ehrenfest Dynamics Using Time-Dependent Density Functional Theory." *J. Phys. Chem. A* 113, 3463-3469. 2009

18. Sergei Tretiak, Christine M. Isborn, Anders M. N. Niklasson, Matt Challacombe. "Representation Independent Algorithms for Molecular Response Calculations in Time-Dependent Self-Consistent Field Theories." *J. Chem. Phys*. 130, 054111. 2009

17. Christine M. Isborn, Xiaosong Li. "Modeling the Doubly Excited State with Time-Dependent Hartree-Fock and Density Functional Theories." *J. Chem. Phys.* 129, 204107. 2008

16. Christine M. Isborn, Svetlana Kilina, Xiaosong Li, Oleg Prezhdo. "Generation of Multiple Excitons in PbSe and CdSe Quantum Dots by Direct Photoexcitation: First-Principles Calculations on Small PbSe and CdSe Clusters." *J. Phys. Chem. C* 112, 18291-18294. 2008

15. David Hrovat, Christine M. Isborn, Bart Kahr, Weston Thatcher Borden. "Internal Dynamics and Optical Rotations Predicted for O_h- and *O*-symmetric Cubanes." *Org. Lett.* 10, 4763-4766. 2008

14. Kacey Claborn, Christine M. Isborn, Werner Kaminsky, Bart Kahr. "Optical Rotation of Achiral Molecules." *Angew. Chem. Int. Ed.* 47, 5706-5717. 2008

13. Joshua A. Davies, Arumugasamy Elangovan, Philip A. Sullivan, Benjamin C. Olbricht, Denise H. Bale, Todd R. Ewy, Christine M. Isborn, Bruce E. Eichinger, Bruce H. Robinson, Philip J. Reid, Xiaosong Li and Larry R. Dalton. "Rational Enhancement of Second-order Nonlinearity: Bis-(4-methoxyphenyl)-*hetero*aryl-amino Donor–Based Chromophores: Design, Synthesis and Electro-optic Activity" *J. Am. Chem. Soc.* 130, 10565-10575. 2008

12. Yoshi Takamoto, Christine M. Isborn, Bruce E. Eichinger, John J. Rehr, Bruce H. Robinson. "Frequency and Solvent Dependence of Nonlinear Optical Properties of Molecules." *J. Phys. Chem. C* 112, 8016-8021. 2008

11. Christine M. Isborn, Xiaosong Li, John C. Tully. "TDDFT Ehrenfest Dynamics: Collisions Between Atomic Oxygen and Graphite Clusters." *J. Chem. Phys*. 126, 134307. 2007

10. Kristin L. Wustholz, Eric D. Bott, Christine M. Isborn, Xiaosong Li, Bart Kahr, Philip J. Reid. "Dispersive Kinetics from Single-Molecules Oriented in Single Crystals of Potassium Acid." *J. Phys. Chem. C* 111, 9146-9156. 2007

9. Christine M. Isborn, Kacey Claborn, Bart Kahr. "The Optical Rotatory Power of Water." *J. Phys. Chem. A* 111, 7800 – 7804. 2007

8. Christine M. Isborn, Amalia Leclerq, Fernando D. Vila, Larry R. Dalton, Jean-Luc Brédas, Bruce E. Eichinger, Bruce H. Robinson. "Comparison of Hyperpolarizabilities Calculated with Various Quantum Mechanical Methods." *J. Phys. Chem. A* 111, 1319-1327. 2007

7. Kacey Claborn, Javier Herreros Cedres, Christine Isborn, Alexey Zozulya, Edgar Weckert, Werner Kaminsky, Bart Kahr. "Optical Rotation of Achiral Pentaerythritol." *J. Am. Chem. Soc.* 128, 14746-14747. 2006

6. Tiffany Kinnibrugh, Sanchali Bhattacharjee, Philip Sullivan, Christine Isborn, Bruce Robinson, Bruce Eichinger. "The Influence of Isomerization on Nonlinear Optical Properties of Molecules." *J. Phys. Chem. B* 110, 13512-13522. 2006

5. Christine M. Isborn, Ernest R. Davidson, Bruce H. Robinson. "*Ab Initio* Diradical/Zwitterionic Polarizabilities and Hyperpolarizabilities in Twisted Double Bonds." *J. Phys. Chem. A* 110, 7189-7196. 2006

4. Bart Kahr, Christine Isborn, Kacey Claborn. "The Role of Chiroptics in Organic Chemistry." *Symmetry: Culture and Science* 16, 4, 423-429. 2005

3. Christine M. Isborn, David A. Hrovat, Weston Thatcher Borden, James M. Mayer, Barry K. Carpenter. "Factors Controlling the Barriers to Degenerate H-atom Transfers." *J. Am. Chem. Soc.* 127, 5794-5795. 2005

2. Christine M. Isborn, David A. Hrovat, Weston Thatcher Borden. "Does Formation of Singlet Propane-1,3-diyl from Propane Deviate from Bond Enthalpy Additivity? Results of *Ab Initio* Calculations That Bear on the Existence of the Benson Barrier to Diradical Ring Closure." *J. Phys. Chem. A* 108, 3024-3029. 2004

1. Claire Castro, Christine M. Isborn, William L. Karney, Michael Mauksch, Paul von Rague Schleyer. "Aromaticity with a Twist: Möbius [4n] Annulenes," *Org. Lett*. 4, 3431-3434. 2002