CONTACT INFORMATION
Department of Chemistry
The Pennsylvania State University
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University Park, PA 16802
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EMPLOYMENT

Assistant Professor of Chemistry (2007-present)
The Pennsylvania State University, University Park, PA, USA

Postdoctoral Researcher with George C. Schatz (2004-2007)
Northwestern University, Evanston, IL, USA

EDUCATION

Rijksuniversiteit Groningen, The Netherlands
Ph.D. in Chemistry (2004)
Thesis: Modelling of Optical Response Properties: Application to Nanostructures
Advisors: Piet Th. van Duijnen and Jaap G. Snijders†
Committee: Evert-Jan Baerends, Benoit Champagne, Koos Duppen

University of Copenhagen, Denmark
M.S. in Chemistry (2000)
B.S. in Chemistry (1998)
Thesis advisors: Kurt V. Mikkelsen and Per-Olof Åstrand

HONORS AND AWARDS

ACS OpenEye Outstanding Junior Faculty Award (2012)
Presidential Early Career Award for Scientists and Engineers, PECASE (2010)
NSF Career Award (2010)
ICCMSE Research Excellence Award (2009)
ICCMSE Young Scientist Prize (2005)
Internationalization Fellowship, Danish Research Agency (2000-2004)

RESEARCH INTEREST

Theoretical Chemistry: Developing and applying electronic structure methods to molecular plasmonics, surface/resonance enhanced vibrational spectroscopy, and nonlinear optical properties.

PUBLICATIONS

73+ papers in international peer review journals. Citations (WoS): 1900+, H-index: 25, checked 08-2012. ResearcherID: B-5132-2008, Full list given at the end.

TEACHING INTEREST	Physical chemistry, quantum chemistry, and computational chemistry
TEACHING EXPERIENCE	Quantum Chemistry I (CHEM 565) Fall 2007,2008,2009,2010,2012 Quantum Chemistry II (CHEM 566) Spring 2009,2010,2013 Physical Chemistry (Chem 452), Spring 2011, Fall 2011 Teaching Assistant in chemistry (Kemi B), University of Copenhagen, Denmark
UNDERGRADUATE STUDENTS	Shannon Noelle Fusina (2008-2011), Victoria Henderson (2009-2010), John M. Rinaldi (2009-2011), Ishita Trivedi(2011-2012), Phil Salant (2011-2012)
GRADUATE STUDENTS	Krista A. Kane (M.S. 2009), Seth Morton (PhD. 2012), Bala Krishna Juluri (PhD. 2011, Supervised jointly with Prof. Tony J. Huang), Daniel Silverstein (2008-), Ebo Ewusi-Annan (M.S. 2010), Justin Moore (2010-), Phillip Weiss (2011-), Dhabih Chulahi (2011-)
POST.DOCS.	Lin Lin Jensen (2008-), John Payton (2010-2012)
PROFESSIONAL AFFILIATION	Member of the American Chemical Society (2004-), Material Research Society (2011-)
PROFESSIONAL SERVICES	Co-organizing "Multiscale Modeling of Optically Responsive Materials" symposium for 2012 Multiscale Materials Modeling, Singapore. Co-organized "Advances in SERS and Molecular Plasmonics" symposium for Fall 2011 ACS Meeting in Denver. Editorial board: Journal of Computational Methods in Science and Engineering(2006-). Computational Chemistry Highlights(2012-). Member: Chemistry Department's Studies Committee, University of Copenhagen (1997,1998), Copenhagen University Evaluation Board of Educations in Chemistry/Physics/Mathematics (1997-1998). Served as reviewer for the following journals: Journal of American Chemical Society, Journal of Chemical Physics, Journal of Computational Chemistry, Journal of Chemical Theory and Computation, Journal of Physical Chemistry A/B/C, Chemical Physics Letter, Chemical Physics, Physical Review B, Physical Review Letters, Nano Letters, Theoretical Chemistry Accounts, ACS Nano, Nature Communications, and others.
OTHER WORK	Contributing author to the ADF program package, www.scm.com Contributing author to the NWChem program package, www.nwchem-sw.org

PUBLICATIONS **Work done at Penn state**.

1. S. Mandal, J. Wang, R. E. Winans, **L. Jensen**, A. Sen
   Quantum Size Effects in the Optical Properties of Ligand Stabilized Aluminum Nanocluster
   J. Am. Chem. Soc, Submitted, 2012
2. Y. B. Zheng, J. L. Payton, T.-B. Song, B. K. Pathem, Y. Zhao, H. Ma, Y. Yang, **L. Jensen**, A. K.-Y. Jen, P. S. Weiss
   Surface-Enhanced Raman Spectroscopy to Probe Photoreaction Pathways and Kinetics of Isolated Reactants on Surfaces: Flat vs. Curved Substrates
   Nano Lett., Submitted, 2012
3. B. K. Pathem, Y. B. Zheng, J. L. Payton, T.-B. Song, B.-C. Yu, J. M. Tour, Y. Yang, **L. Jensen**, P. S. Weiss
   Effect of Tether Conductivity on the Efficiency of Photoisomerization of Azobenzene-Functionalized Molecules on Au{111}
   J. Phys. Chem. Lett., Submitted, 2012
4. B. K. Pathem, Y. B. Zheng, S. Morton, M. Å. Petersen, C.-H. Chung, Y. Yang, **L. Jensen**, M. B. Nielsen, P. S. Weiss
   Photoreaction of Matrix-Isolated Dihydroazulene-Functionalized Molecules on Au{111}
   Nano Lett., Submitted, 2012
5. A. N. Giordano, S. M. Morton, **L. Jensen**, B. J. Lear
   A Direct Test of the Equivalency of Dynamic IR and Dynamic Raman Spectroscopies as Techniques for Observing Ultrafast Molecular Dynamics
   J. Phys. Chem. A, Submitted, 2012
6. J. E. Moore, S. M. Morton, **L. Jensen**
   Importance of Correctly Describing Charge-transfer Excitations for Understanding the Chemical Effect in SERS
   J. Phys. Chem. Lett., Submitted, 2012
7. J. L. Payton, S. M. Morton, J. E. Moore, **L. Jensen**
   A Discrete Interaction Model/Quantum Mechanical Method for Simulating Surface-Enhanced Raman Spectroscopy
   J. Chem. Phys., **133**, 214103, 2012
8. K. M. Schmid, **L. Jensen**, S. T. Phillips
   A Self-Immolative Spacer that Enables Tunable Controlled Release of Phenols under Neutral Conditions
   J. Org. Chem., **77**, 4363-4374, 2012
9. Q. Hao, B. Wang, J. Bossard, B. Kiraly, Y. Zeng, I.-K. Chiang, **L. Jensen**, D. Werner, T. J. Huang
   Surface-Enhanced Raman Scattering Study on Graphene Coated Metallic Nanostructure Substrates
   J. Phys. Chem. C., **116**, 7249-7254, 2012
   Featured on the cover.

10. D. W. Silverstein, **L. Jensen**
Vibronic Coupling Simulations for Linear and Nonlinear Optical Processes: Simulation Results
J. Chem. Phys., **136**, 064110, 2012

11. D. W. Silverstein, **L. Jensen**
Vibronic Coupling Simulations for Linear and Nonlinear Optical Processes: Theory
J. Chem. Phys., **136**, 064111, 2012

12. S. M. Morton, **L. Jensen**
A Discrete Interaction Model/Quantum Mechanical Method to Describe the Interaction of Metal Nanoparticles and Molecular Absorption
J. Chem. Phys., **135**, 134103, 2011

13. C. B. Milojevich, D.W. Silverstein, **L. Jensen**, J. P. Camden
Probing Two-Photon Properties of Molecules: Large Non-Condon Effects Dominate the Resonance Hyper-Raman Scattering of Rhodamine 6G
J. Am. Chem. Soc., **133**, 14590-14592, 2011

14. Y. B. Zheng, J. L Payton, C. H. Chung, R. Liu, S. Cheunkar, B. K. Pathem, Y. Yang, **L. Jensen**, P. S. Weiss
Surface-Enhanced Raman Spectroscopy to Probe Reversible Photoswitchable Azobenzene in Controlled Nanoscale Environments
Nano Lett. **11**, 3447-3452, 2011

15. B. K. Juluri, N. Chaturvedi, Q. Z. Hao, M. Q. Lu, D. Velogol, **L. Jensen**, T. J. Huang
Scalable Manufacturing of Plasmonic Nanodisk Dimers and Cups Nanostructures Using Salting-Out Quenching Method and Colloidal Lithography
ACS Nano, **5**, 5838-5847, 2011

16. Q. Hao, Y. Zheng, B. K. Juluri, X. D. Wang, B. Kiraly, I.K. Chiang, **L. Jensen**, D. H. Werner, V. H. Crespi, T. J. Huang
Metallic Membranes with Subwavelength Complementary Patterns: Distinct Substrates for Surface-Enhanced Raman Scattering
ACS Nano, **5**, 5472-5477, 2011

17. E. H. Witlicki, C. Johnsen, S. W. Hansen, D. W. Silverstein, V. J. Bottomley, J. O. Jeppesen, E. W. Wong, **L. Jensen**, A. H. Flood
Molecular Logic Gates Using Surface-Enhanced Raman-Scattered Light
J. Am. Chem. Soc., **133**, 7288-7291, 2011

18. S. M. Morton, D. W. Silverstein, **L. Jensen**
Theoretical Studies of Plasmonics using Electronic Structure Theory
Chem. Rev, **111**, 3962-3994, 2011
Invited review article.

19. C. P. Bennett, D. W. Silverstein, **L. Jensen**, J. P. Camden
Probing One-Photon Inaccessible Electronic States with High Sensitivity: Wavelength Scanned Surface Enhanced Hyper-Raman Scattering
Chem. Phys. Chem., **12**, 101-103, 2011

20. N. E. Motl, E. Ewusi-Annan, I. T. Sines, **L. Jensen**, R. E. Schaak
Au-Cu Alloy Nanoparticles with Tunable Compositions and Plasmonic Properties: Experimental Determination of Composition and Correlation with Theory
J. Phys. Chem C, **114**, 19263-19269, 2010

21. Q. Hao, B. K. Juluri, Y. B. Zheng, B. Wang, **L. Jensen**, V. Crespi, P. C. Eklund, T. J. Huang
Effects of Intrinsic Fano Interference on Surface Enhanced Raman Spectroscopy: Comparison between Platinum and Gold
J. Phys. Chem. C. **114**, 18059-18066, 2010
Featured on the cover.

22. D. W. Silverstein, **L. Jensen**
Understanding the Resonance Raman Scattering of Donor-Acceptor Complexes using Long-Range Corrected DFT
J. Chem. Theo. Comp., **6**, 28452855, 2010

23. S. M. Morton, **L. Jensen**
A Discrete Interaction Model/Quantum Mechanical Method for Describing Response Properties of Molecules Adsorbed on Metal Nanoparticles
J. Chem. Phys., **133**, 074103, 2010

24. Y. B. Zheng, B. K. Juluri, L. L. Jensen, D. Ahmed, M. Lu, **L. Jensen**, T. J. Huang
Dynamically Tuning Plasmon–Exciton Coupling in Arrays of Nanodisk–J-Aggregate Complexes
Adv. Mat., **22**, 3603, 2010
Featured on the cover.

25. D. W. Silverstein, **L. Jensen**
Assessment of the Accuracy of Long-Range Corrected Functionals for Describing the Electronic and Optical Properties of Silver Clusters
J. Chem. Phys., **132**, 194302, 2010

26. E. H. Witlicki, S. S. Andersen, S. W. Hansen, J. O. Jeppesen, E. W. Wong, **L. Jensen**, A. H. Flood
Turning on Resonant SERRS Using the Chromophore-Plasmon Coupling Created by Host-Guest Complexation at a Plasmonic Nanoarray
J. Am. Chem. Soc, **132**, 6099-6107, 2010

27. K. A. Kane, **L. Jensen**
Calculation of Absolute Resonance Raman Intensities: Vibronic Theory vs. Short-time Approximation
J. Phys. Chem. C, **114**,5540-5546, 2010, Invited Article: Barbara J. Garrison Special issue.

28. B. K. Juluri, M. Lu, Y. B. Zheng, T. J. Huang, **L. Jensen**
Coupling between Molecular and Plasmonic Resonances: Effect of Molecular Absorbance
J. Phys. Chem. C, **113**, 18499-18503, 2009

29. **L. Jensen**, N. Govind
Excited States of DNA Base Pairs Using Long-Range Corrected Time-Dependent Density Functional Theory
J. Phys. Chem A, **113**, 9761-9765, 2009,
Reply to comment: J. Phys. Chem. A, **113**, 11095, 2009.

30. E. H. Witlicki, S. W. Hansen, M. Christensen, T. S. Hansen, S. D. Nygaard, J. O. Jeppesen, E. W. Wong, **L. Jensen**, A. H. Flood
Determination of Binding Strengths of a Host-Guest Complex Using Resonance Raman Scattering
J. Phys. Chem. A, **113**, 9450-9457, 2009

31. L. L. Jensen, **L. Jensen**
An Atomistic Electrodynamics Model for Optical Properties of Silver Nanoclusters
J. Phys. Chem. C, **113**, 15182-15190, 2009

32. S. M. Morton, E. Ewusi-Annan, **L. Jensen**
Controlling the Non-Resonant Chemical Mechanism of SERS Using a Molecular Photoswitch
Phys. Chem. Chem. Phys., **11**, 7424-7429, 2009

33. N. Govind, M. Valiev, **L. Jensen**, K. Kowalski
Excitation Energies of Zinc Porphyrin in Aqueous Solution Using Long-Range Corrected Time-Dependent Density Functional Theory
J. Phys. Chem, A, **113**, 6041-6043, 2009

34. B. K. Juluri, S.-C. S. Lin, T. R. Walker, T. J. Huang, **L. Jensen**
Propagation of Designer Surface Plasmons in Structured Conductor Surfaces with Parabolic Gradient Index
Opt. Express, **17**, 2997–3006, 2009

35. Y. B. Zheng, L. L. Jensen, W. Yan, T. Walker, B. K. Juluri, **L. Jensen**, T. J. Huang
Chemically Tuning the Localized Surface Plasmon Resonances of Gold Nanostructure Arrays
J. Phys. Chem. C, **113**, 7019–7024, 2009

36. S. M. Morton, **L. Jensen**
Understanding the Molecule-Surface Chemical Coupling in SERS
J. Am. Chem. Soc, **131**, 4090-4098, 2009

37. **L. Jensen**
Surface-Enhanced Vibrational Raman Optical Activity: A Time-Dependent Density Functional Theory Approach
J. Phys. Chem. A, **113**, 4437–4444, 2009
Invited Article: George C. Schatz Special issue.

38. Y. B. Zheng, Y.-W. Yang, **L. Jensen**, L. Fang, B. K. Juluri, A. H. Flood, P. S. Weiss, J. F. Stoddart, T. J. Huang
Active Molecular Plasmonics: Controlling Plasmon Resonances with Molecular Switches
Nano Lett., **9**, 819-825, 2009
Highlighted in Nature Materials.

39. L. L. Jensen, **L. Jensen**
Electrostatic Interaction Model for the Calculation of the Polarizability of Large Noble Metal Nanoclusters
J. Phys. Chem. C, **112**, 15697–15703, 2008
Featured on the cover.

40. B. K. Juluri, Y. B. Zheng, D. Ahmed, **L. Jensen**, T. J. Huang,
Effects of Geometry and Composition on Charge-Induced Plasmonic Shifts in Gold Nanoparticles
J. Phys. Chem. C, **112** , 7309 -7317, 2008

Based on work prior to Penn State

41. M. Sonntag, J. Klingsporn, L. Garibay, J. Roberts, J. Dieringer, T. Seideman, K. Scheidt, L. Jensen, G. C. Schatz, R. P. Van Duyne
Single Molecule Tip Enhanced Raman Spectroscopy
J. Phys. Chem. C, **116**, 478-483, 2012

42. N. Valley, **L. Jensen**, J. Autschbach, G. C. Schatz
Theoretical Studies of Surface Enhanced Hyper-Raman Spectroscopy: The Chemical Enhancement Mechanism
J. Chem. Phys., **133**, 054103, 2010

43. H. S. Smalø, P.-O. Åstrand, **L. Jensen**
Nonmetallic Electronegativity Equalization and Point-Dipole Interaction Model Including Exchange Interactions for Molecular Dipole Moments and Polarizabilities
J. Chem. Phys., **131**, 044101, 2009

44. **L. Jensen**, P.-O. Åstrand, K. V. Mikkelsen
Molecular Mechanics Interaction Models for Optical Electronic Properties
J. Comp. Theo. Nanoscience, **6**, 270291 (2009)
Invited review article.

45. **L. Jensen**, C. M. Aikens, G. C. Schatz
Electronic Structure Methods for Studying Surface-Enhanced Raman Scattering
Chem. Soc. Rev., **37**, 1061 - 1073, 2008

46. **L. Jensen**, J. Autschbach, M. Krykunov, G. C. Schatz
Resonance Vibrational Raman Optical Activity: A Time-Dependent Density Functional Theory Approach
J. Chem. Phys., **127**, 134101, 2007

47. J. Zhao, **L. Jensen**, J. Sung, S. Zou, G. C. Schatz, T. P. van Duyne
Interaction of Plasmon and Molecular Resonances for Rhodamine 6G Adsorbed on Silver Nanoparticles
J. Am. Chem. Soc., **129**, 7647-7656, 2007

48. **L. Jensen**, L. L. Zhao, G. C. Schatz
Size-Dependence of the Enhanced Raman Scattering of Pyridine Adsorbed on Ag_n ($n = 2-8, 20$) Clusters
J. Phys. Chem. C., **111**, 4756-4764, 2007

49. **L. Jensen**, P.-O. Åstrand, K. V. Mikkelsen
Microscopic Polarization in Ropes and Films of Aligned Carbon Nanotubes
J. Comput. Meth. Sci. Eng., **6**, 353-364, 2006

50. **L. Jensen**, M. Swart, P. Th. van Duijnen, J. Autschbach
The CD-Spectrum of $[Co(en)_3]^{3+}$ in Solution Using the Discrete Solvent Reaction Field Model
Int. J. Quant. Chem., **106**, 2479-2488, 2006

51. L. L. Zhao, **L. Jensen**, G. C. Schatz
Surface-Enhanced Raman Scattering of Pyrazine at the Junction Between Two Ag_{20} Nanoclusters
Nano Lett., **6**, 1229-1234, 2006

52. C. R. Jacob, J. Neugebauer, **L. Jensen**, L. Visscher
Comparison of Frozen-Density Embedding and Discrete Reaction Field Solvent Models for Molecular Properties
Phys. Chem. Chem. Phys., **8**, 2349-2359, 2006

53. **L. Jensen**, G. C. Schatz
Resonance Raman Scattering of Rhodamine 6G as Calculated Using Time-Dependent Density Functional Theory
J. Phys. Chem. A, **110**, 5973-5977, 2006
Among the most-accessed articles: April-June, 2006

54. L. L. Zhao, **L. Jensen**, G. C. Schatz
Pyridine – Ag_{20} Cluster: A Model System for Studying Surface-Enhanced Raman Scattering
J. Am. Chem. Soc., **128**, 2911-2919, 2006

55. J. Autschbach, **L. Jensen**, G. C. Schatz, Y. C. E. Tse, M. Krykunov
Time-Dependent Density Functional Calculations of Optical Rotatory Dispersion Including Resonance Wavelengths as a Potentially useful Tool for Determining Absolute Configurations of Chiral Molecules
J. Phys. Chem. A, **110**, 2461-2473, 2006

56. J. Kongsted, T. B. Pedersen, **L. Jensen**, A. E. Hansen, K. V. Mikkelsen
Coupled Cluster and Density Functional Theory Studies of the Vibrational Contribution to the Optical Rotation of (S)-Propylene Oxide
J. Am. Chem. Soc., **128**, 976-982, 2006

57. **L. Jensen**, L. L. Zhao, J. Autschbach, G.C. Schatz
Theory and Method for Calculating Resonance Raman Scattering from Resonance Polarizability Derivatives
J. Chem. Phys., **123**, 174110, 2005

58. **L. Jensen**, P. Th. van Duijnen
The First Hyperpolarizability of p-Nitroaniline in 1,4-dioxane: A Quantum Mechanical / Molecular Mechanics Study
J. Chem. Phys., **123**, 074307, 2005

59. T. Hansen, **L. Jensen**, P.-O. Åstrand, K. V. Mikkelsen
Frequency-Dependent Polarizabilities of Amino Acids as Calculated by an Electrostatic Interaction Model
J. Chem. Theo. Comp., **1**, 626-633, 2005

60. **L. Jensen**, J. Autschbach, G. C. Schatz
Finite Lifetime Effects on the Polarizability Within Time-Dependent Density-Functional Theory
J. Chem. Phys., **122**, 224115, 2005

61. **L. Jensen**, P. Th. van Duijnen
Refractive Index and Third-Order Nonlinear Susceptibility of C-60 in the Condensed Phase Calculated with the Discrete Solvent Reaction Field Model
Int. J. Quant. Chem., **102**, 612-619, 2005

62. **L. Jensen**, M. Swart, P. Th. van Duijnen
Microscopic and Macroscopic Polarization Within a Combined Quantum Mechanics and Molecular Mechanics Model
J. Chem. Phys., **122**, 034103, 2005

63. **L. Jensen**, P.-O. Åstrand, K. V. Mikkelsen
The Static Second Hyperpolarizability of Fullerenes and Carbon Nanotubes
J. Phys. Chem. A, **108**, 8795-8800, 2004

64. M. van Faassen, **L. Jensen**, J. A. berger, P. L. de Boeij
Size-Scaling of the Polarizability of Tubular Fullerenes Investigated with Time-Dependent (Current-)-Density-Functional Theory
Chem. Phys. Lett., **395**, 274-278, 2004

65. **L. Jensen**, P.-O. Åstrand, K. V. Mikkelsen
Microscopic and Macroscopic Polarization in C_{60} Fullerene Clusters as Calculated by an Electrostatic Interaction Model
J. Phys. Chem. B, **108**, 8226-8233, 2004

66. **L. Jensen**, P. Th. van Duijnen, J. G. Snijders
A Discrete Solvent Reaction Field Model for Calculating Frequency-Dependent Hyperpolarizabilities of Molecules in Solution
J. Chem. Phys., **119**, 12998-13006, 2003

67. **L. Jensen**, P. Th. van Duijnen, J. G. Snijders
A Discrete Solvent Reaction Field Model for Calculating Molecular Linear Response Properties in Solution
J. Chem. Phys., **119**, 3800-3809, 2003

68. R.-H. Xie, **L. Jensen**, G. W. Bryant, J. J. Zhao, V. H. Smith Jr.
Structural, Electronic, and Magnetic Properties of Heterofullerene $C_{48}B_{12}$
Chem. Phys. Lett., **375**, 445-451, 2003

69. **L. Jensen**, P.-O. Åstrand, K. V. Mikkelsen
Saturation of the Third-Order Polarizability of Carbon Nanotubes Characterized by a Dipole Interaction Model
Nano Lett., **3**, 661-665,2003

70. R.-H. Xie, G. W. Bryant, **L. Jensen**, J. J. Zhao, V. H. Smith Jr.
First-Principles Calculations of Structural, Electronic, Vibrational and Magnetic Properties of C_{60} and $C_{48}N_{12}$: A Comparative Study
J. Chem. Phys., **118**, 8621-8635, 2003

71. **L. Jensen**, K. O. Sylvester-Hvid, K. V. Mikkelsen, P.-O. Åstrand
A Dipole Interaction Model for the Molecular Second Hyperpolarizability
J. Phys. Chem. A, **107**, 2270-2276, 2003

72. **L. Jensen**, P. Th. van Duijnen, J. G. Snijders
A Discrete Solvent Reaction Field Model Within Density Functional Theory
J. Chem. Phys., **118**, 514-521, 2003

73. **L. Jensen**, M. Swart, P. Th. van Duijnen, J. G. Snijders
Medium Perturbations on the Molecular Polarizability Calculated Within a Localized Dipole Interaction Model
J. Chem. Phys., **117**, 3316-3320, 2002

74. **L. Jensen**, P. Th. van Duijnen, J. G. Snijders, D. P. Chong
Time-Dependent Density Functional Study of the Static Second Hyperpolarizability of BB-, NN- and BN-substituted C_{60}
Chem. Phys. Lett., **359**, 524-529, 2002

75. **L. Jensen**, P.-O. Åstrand, A. Osted, J. Kongsted, K. V. Mikkelsen
Polarizability of Molecular Clusters as Calculated by a Dipole Interaction Model
J. Chem. Phys., **116**, 4001-4010, 2002

76. T. L. C. Jansen, M. Swart, **L. Jensen**, P. Th. van Duijnen, J. G. Snijders, K. Duppen
Collision Effects in the Nonlinear Raman Response of Liquid Carbon Disulfide
J. Chem. Phys., **116**, 3277-3285, 2002

77. J. Kongsted, A. Osted, **L. Jensen**, P.-O. Åstrand, K. V. Mikkelsen
Frequency-Dependent Polarizability of Boron Nitride Nanotubes: A Theoretical Study
J. Phys. Chem. B, **105**, 10243-10248, 2001

78. **L. Jensen**, P.-O. Åstrand, K. V. Mikkelsen
An Atomic Capacitance-Polarizabililty Model For The Calculation of Molecular Dipole Moments and Polarizabilities
Int. J. Quant. Chem., **84**, 513-522, 2001

79. **L. Jensen**, O. H. Schmidt, K. V. Mikkelsen, P.-O. Åstrand
Static and Frequency-Dependent Polarizability Tensors for Carbon Nanotubes
J. Phys. Chem. B, **104**, 10462-10466, 2000

80. **L. Jensen**, P.-O. Åstrand, K. O. Sylvester-Hvid, K. V. Mikkelsen
Frequency-Dependent Molecular Polarizability Calculated Within an Interaction Model
J. Phys. Chem. A, **104**, 1563-1569, 2000

BOOK CHAPTERS

1. John L. Payton, Seth M. Morton, **L. Jensen**
First-Principles Simulations of Near Field Effects, in Agio, M. and Alu, A. (editors), "Optical Antennas", Cambridge University Press, ISBN: 9781107014145 , 2012.

2. N. Valley, **L. Jensen**, J. Autschbach, G. C. Schatz
Calculating the Raman and HyperRaman Spectra of Large Molecules and Molecules Interacting with Nanoparticles, in Reimers, J. (editor), "Computational Methods for Large Systems", Wiley, ISBN: 978-0-470-48788-4, 2011.

3. P.Th. van Duijnen, M. Swart and **L. Jensen**
The Discrete Reaction Field approach for calculating solvent effects
in "Solvation Effects on Molecules and Biomolecules: Computational Methods and Applications"; Springer Series "Challenges and Advances in Computational Chemistry and Physics", Vol. 6; 39102, Edited by S. Canuto, Springer, 2008

4. **L. Jensen**, P. Th. van Duijnen
The Discrete Solvent Reaction Field model: A Quantum mechanics / Molecular Mechanics Model for Calculating Nonlinear Optical Properties of Molecules in Condensed Phase
in "Atoms, Molecules and Clusters in Electric Fields. Theoretical Approaches to the Calculation of Electric Polarizability". Edited by G. Maroulis, Imperial College Press, 2006, ISBN 1-86094-676-3
5. R.-H. Xie, Q. Rao, **L. Jensen**
Nonlinear Optics of Fullerenes and Carbon Nanotubes
in "Encyclopedia of Nanoscience and Nanotechnology", Edited by H. S. Nalwa, American Scientific Publisher, Vol. 8, 67-99. 2004

OTHER PUBLICATIONS

1. M. A. Ratner, R. P. Van Duyne, **L. Jensen**, D. Troya
Tribute to George C. Schatz
J. Phys. Chem. A, 113, 37093710, 2009
2. **L. Jensen**
Molekylær Plasmonik som Ultrafølsomme Sensorer
Dansk Kemi, **89**, 1, 36–38,2007 (in Danish)
3. **L. Jensen**
Local Field Effects on Nonlinear Optical Properties: Insights from Combined Quantum Mechanical and Molecular Mechanics Models
in "Advances in computational methods in sciences and engineering" Edited by T. Simos and G. Maroulis, VSP BV, Vol. 4, 958-960, 2005, ISBN 90-6764-441-2
ICCMSE 2005 Conference Abstract

INVITED TALKS

1. "TBD", CECAM Workshop: "Stabilized Metal Nanoparticles, Recent Computational Advances and Present Challenges", Helsinki, Finland, Scheduled June 4-June 6 2013.
2. "TBD", William and Mary, Williamsburg, VA, Scheduled November 2012.
3. "Plasmon-Enhanced Chiroptical Properties: A Combined Atomistic Electrodynamics-Quantum Mechanics Model", CECAM Workshop: "Vibrational Optical Activity: Interplay of Theory and Experiment", Pisa, Italy, Scheduled September 23-27, 2012. (Plenary Speaker)
4. "Understanding the Molecule-Plasmon Coupling", 244th American Chemical Society Meeting, Philadelphia, PA USA., Scheduled August 19-23, 2012.
5. "Understanding the Plasmon Molecule Coupling", TSRC Workshop: Nanomaterials: Theory and Computation, Telluride, CO, July 16-19, 2012.
6. "A Combined Atomistic Electrodynamics-Quantum Mechanics Model for Simulating Plasmon Enhanced Spectroscopy", International Conference on Theoretical and High Performance Computational Chemistry, Nanjing, China, July 8 -11, 2012.
7. "Quantum Effects in Surface-Enhanced Spectroscopy", GRC Noble Metal Nanoparticle, Mount Holyoke College, MA, June 17-22, 2012.

8. “Understanding the Molecule-Plasmon Coupling ”, CNSI, UCLA, May 9, 2012.
9. “Understanding The Molecule-Plasmon Coupling”, Greater Boston Area Theoretical Chemistry Lecture, Boston University, MIT, Harvard University, MA, March, 31, 2012.
10. “Understanding the Molecule-Plasmon Coupling”, Argonne National Laboratory, IL, March 6, 2012.
11. “Understanding the Molecule-Plasmon Coupling”, Northwestern University, Evanston, IL, March 12, 2012.
12. ”Understanding the Molecule-Plasmon Coupling”, Indiana University, Bloomington, IN, March 8, 2012.
13. ”Understanding the Molecule-Plasmon Coupling”, University of Pennsylvania, Philadelphia, PA, February 9, 2012.
14. ”Understanding the Molecule-Plasmon Coupling”, workshop Nanophotonics and Nanoplasmonics, Bangalore, India, January 9-12, 2012
15. ”Simulating Vibronic Effects in Two-Photon Absorption and Resonance Hyper-Raman Scattering”, Materials Research Society Meeting, Boston, MA, November 28-December 2, 2011.
16. ”New Computational Tools for Understanding Molecular Plasmonics”, UC Irvine, Irvine, CA, November 10, 2011.
17. ”Understanding Molecular Plasmonics Using TDDFT”, Gordon Research Conference: Time-Dependent Density-Functional Theory, Biddeford, ME, August 14-19, 2011.
18. ”Understanding the Molecule-Plasmon Coupling”, University of Florida, Gainesville, FL, October 26, 2010.
19. ”Theoretical Studies of SERS Using Electronic Structure Theory and Other Things...”, Gordon Research Conference on Plasmonics, Colby College, ME, June 2010.
20. ”Understanding the Molecule-Plasmon Coupling”. Chemistry for the Next Generation by the Next Generation, Northwestern University, Evanston, IL, May 28-30, 2010.
21. ”Understanding the Molecule-Plasmon Coupling, UC Irvine, Irvine, CA, May 13, 2010.
22. ”On the Chemical Coupling in SERS”, ICCMSE, Rhodes, Greece, September 29-October 4, 2009. (Keynote Speaker)
23. “Long-Range Corrected Functionals in NWChem”, Penn State University, University Park, PA, October 12, 2009.
24. “Surface-Enhanced Vibrational Spectroscopy: Insights From Theory”, Indiana University of Pennsylvania, Indiana, PA, March 28, 2008.
25. “Surface-Enhanced Raman Scattering: Mechanistic Insights from Molecules Interacting with Small Metal Clusters”, Texas A&M University, College Station, TX, January 12, 2007.
26. “Surface-Enhanced Raman Scattering: Mechanistic Insights from Molecules Interacting with Small Metal Clusters”, Penn State University, University Park, PA, December 07, 2006.

27. "Understanding Surface-Enhanced Raman Scattering using Electronic Structure Methods", University of Buffalo, Buffalo, NY, February 2006.
28. "Understanding Surface-Enhanced Raman Scattering using Electronic Structure Methods", The Norwegian University of Science and Technology, Trondheim, Norway, October 2005.
29. "Understanding Surface-Enhanced Raman Scattering using Electronic Structure Methods", University of Copenhagen, Denmark, October 2005.
30. "Understanding Surface-Enhanced Raman Scattering using Electronic Structure Methods", Rijksuniversiteit Groningen, The Netherlands, October 2005.
31. "Understanding Surface-Enhanced Raman Scattering using Electronic Structure Methods", Vrije Universiteit Amsterdam, The Netherlands, October 2005.
32. "Local Field Effects on Nonlinear Optical Properties: Insights From Combined Quantum Mechanical and Molecular Mechanics Models", ICCMSE, Loutraki, Korinthos, Greece, October 2005.
33. "Non-linear Optical Properties of Carbon Nanostructures: From Molecules to Materials", Rijksuniversiteit Groningen, The Netherlands, September 2004.
34. "Non-linear Optical Properties of Carbon Nanostructures: From Molecules to Materials", University of Copenhagen, Denmark, September 2004.
35. "Non-linear Optical Properties of Carbon Nanostructures: From Molecules to Materials", University of Aarhus, Denmark, September 2004.
36. "Non-linear Optical Properties of Carbon Nanostructures: From Molecules to Materials", University of Buffalo, Buffalo, NY, March 2004.
37. "Polarizabilities and Second Hyperpolarizabilities of Carbon Nanotubes and C60 Fullerene Clusters Calculated by an Electrostatic Interaction Model", A Coastal Voyage in Quantum Chemistry, The University of Tromsø, Norway, September 2003.
38. "Non-linear Optical Properties of Carbon Nanostructures: From Molecules to Materials", Northwestern University, Evanston, IL, March 2003.
39. "A Discrete Solvent Reaction Field Model for Calculating Molecular Response Properties in Solution", Norwegian University of Science and Technology, Trondheim, Norway, September 2001.
40. "An Interaction Model for Describing the Frequency-Dependent Polarizability", Rijkuniversiteit Groningen, The Netherlands, October 1999.

CONTRIBUTED TALKS

1. "Combined Atomistic Electrodynamic-Quantum Mechanical Method for Simulating Plasmon Enhanced Molecular Properties", 244th American Chemical Society Meeting, Philadelphia, PA USA., Scheduled August 19-23, 2012.
2. "Nanoparticle Enhanced Spectroscopy", 243rd ACS National Meeting, San Diego, CA, March 25-29, 2012.
3. "Coupling Molecular and Plasmonic Excitations", 243nd American Chemical Society Meeting, San Diego, CA, March 25-29, 2012.

4. "Understanding the Molecule-Plasmon Coupling", 242nd American Chemical Society Meeting, Denver, CO, August 28-September 1, 2011.
5. "Advances in SERS and Molecular Plasmonics", 242nd American Chemical Society Meeting, Denver, CO, August 29-September 1, 2011.
6. "Resonance Raman Scattering of Charge-Transfer Complexes Using Long-Range Corrected DFT", 240th American Chemical Society Meeting, Boston, MA, April 22-26, 2010.
7. "Understanding the Molecule-Surface Chemical Coupling in SERS", 238th American Chemical Society Meeting, Washington DC, August, 2009.
8. "An Electrostatic Interaction Model for Polarizability of Metal Nanoparticles", 237th American Chemical Society Meeting, Salt Lake City, UT, March, 2009.
9. "Understanding the Molecule-Surface Chemical Coupling in SERS", George C. Schatz 60th Birthday Conference, Northwestern University, Evanston, IL, April, 2009.
10. "Surface-Enhanced Vibrational Spectroscopy: Insights from TDDFT", 235th American Chemical Society Meeting, New Orleans, LA, April 2008.
11. "TDDFT Studies of Resonance Raman and Resonance Vibrational Raman Optical Activity", 235th American Chemical Society Meeting, New Orleans, LA, April 2008.
12. "Resonance Vibrational Raman Optical Activity within Time-Dependent Density Functional Theory", 233rd American Chemical Society Meeting, Chicago, IL, March 2007.
13. "Raman spectroscopy: New Challenges for Theory", 232nd American Chemical Society Meeting, San Francisco, CA, September 2006.
14. "A Discrete Solvent Reaction Field Model for Calculating Molecular Response Properties in Solution", 10th International Conference on the Application of Density Functional Theory in Chemistry and Physics, Brussels, Belgium, September 2003.
15. "A Discrete Solvent Reaction Field Model for Calculating Molecular Response Properties in Solution", The Bi-Annual Meeting of Materials Science Centre, Vlieland, The Netherlands, April 2003.
16. "A Discrete Solvent Reaction Field Model for Calculating Molecular Response Properties in Solution", Minisymposium, Computational Methods in Quantum Chemistry, The University of Tromsø , Norway, June 2002.

FUNDING

Agency: National Science Foundation
Principal Investigator: Lasse Jensen
Project Title: CAREER: Theoretical Studies of Optical Properties of Molecules Near Metal Nanostructures
Award Dates: 1/1/2010-12/31/2014
Total Costs: $613,047

Agency: National Science Foundation, CaSTL
Principal Investigator: V. Ara Apkarian, UC Irvine
Co-Investigators: Lasse Jensen
Project Title: : CaSTL: Modeling Surface-Enhanced Raman Optical Activity
Award Dates: 05/01/2012-04/31/2013
Total Costs: $55,087 (My Share)

Agency: AFORS
Principal Investigator: David Rauh, EIC Laboratories, Inc
Co-Investigators: Lasse Jensen
Project Title: STTR: Tools for Modeling and Simulation of Molecular and Nanomaterials for Optically Responsive Devices
Award Dates: 06/15/2010-03/14/2011
Total Costs: $50,000 (My Share)

Agency: National Science Foundation, MRSEC Seed Grant
Principal Investigator: T. J. Huang
Co-Investigators: Lasse Jensen
Project Title: Understanding and Harvesting Biomimetic Molecular Motors for Active Plasmonics
Award Dates: 1/1/2008-5/31/2009
Total Costs: $50,000 funded joint student

Agency: TERAGRID
Principal Investigator: Lasse Jensen
Project Title: Resonance Raman of Molecules Using Long-Range Corrected Functionals
Award Dates: 9/25/2009- 9/25/2010
Total Costs: 30.000 CPU Hours

Agency: EMSL
Principal Investigator: Lasse Jensen
Project Title: Optical Properties of Silver Nano-Quantum-Dots Using Long-Range Corrected TDDFT
Award Dates: 10/1/2009- 9/31/2010
Total Costs: 20.000 CPU Hours

Agency: EMSL
Principal Investigator: Lasse Jensen
Project Title: Theoretical Studies of Enhanced Optical Properties of Molecule-Metal Clusters
Award Dates: 10/1/2010- 9/31/2011
Total Costs: 50.000 CPU Hours