Lasse Jensen

List of Publications by Year in descending order

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145 papers	9,233 citations	41344 49 h-index	42399 92 g-index
150 all docs	150 docs citations	150 times ranked	8706 citing authors

#	Article	IF	Citations
1	Development of magnetic nanoparticles for the intracellular delivery of miR-148b in non-small cell lung cancer. Biomedical Engineering Advances, 2022, 3, 100031.	3.8	9
2	Local-Field Effects in Linear Response Properties within a Polarizable Frozen Density Embedding Method. Journal of Chemical Theory and Computation, 2022, 18, 380-393.	5.3	7
3	Surface-enhanced hyper-Raman scattering of Rhodamine 6G isotopologues: Assignment of lower vibrational frequencies. Journal of Chemical Physics, 2021, 154, 034703.	3.0	2
4	Monitoring Reaction Intermediates in Plasma-Driven SO₂, NO, and NO₂ Remediation Chemistry Using In Situ SERS Spectroscopy. Analytical Chemistry, 2021, 93, 6421-6427.	6.5	8
5	A discrete interaction model/quantum mechanical method for simulating surface-enhanced Raman spectroscopy in solution. Journal of Chemical Physics, 2021, 154, 224705.	3.0	8
6	Comparison of thermoresponsive Diels-Alder linkers for the release of payloads from magnetic nanoparticles via hysteretic heating. Jcis Open, 2021, 4, 100034.	3.2	6
7	2020 JCP Emerging Investigator Special Collection. Journal of Chemical Physics, 2021, 155, 230401.	3.0	1
8	JCP Emerging Investigator Special Collection 2019. Journal of Chemical Physics, 2020, 153, 110402.	3.0	2
9	Chemical physics of materials. Journal of Chemical Physics, 2020, 153, 100402.	3.0	0
10	Quantifying the enhancement mechanisms of surface-enhanced Raman scattering using a Raman bond model. Journal of Chemical Physics, 2020, 153, 224704.	3.0	11
11	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
12	Alternating magnetic field mediated release of fluorophores from magnetic nanoparticles by hysteretic heating. Journal of Colloid and Interface Science, 2020, 571, 348-355.	9.4	9
13	Monitoring Local Electric Fields using Stark Shifts on Napthyl Nitrile-Functionalized Silicon Photoelectrodes. Journal of Physical Chemistry C, 2020, 124, 17000-17005.	3.1	4
14	A Benchtop Method for Appending Protic Functional Groups to Nâ€Heterocyclic Carbene Protected Gold Nanoparticles. Angewandte Chemie, 2020, 132, 7655-7660.	2.0	9
15	Interpreting the chemical mechanism in SERS using a Raman bond model. Journal of Chemical Physics, 2020, 152, 024126.	3.0	25
16	A Benchtop Method for Appending Protic Functional Groups to Nâ€Heterocyclic Carbene Protected Gold Nanoparticles. Angewandte Chemie - International Edition, 2020, 59, 7585-7590.	13.8	31
17	Resolving Molecular Structures with High-Resolution Tip-Enhanced Raman Scattering Images. ACS Nano, 2019, 13, 9342-9351.	14.6	29
18	Polarizable Frozen Density Embedding with External Orthogonalization. Journal of Chemical Theory and Computation, 2019, 15, 6588-6596.	5.3	8

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19	Measuring Local Electric Fields and Local Charge Densities at Electrode Surfaces Using Graphene-Enhanced Raman Spectroscopy (GERS)-Based Stark-Shifts. ACS Applied Materials & Interfaces, 2019, 11, 36252-36258.	8.0	7
20	Atomistic electrodynamics simulations of plasmonic nanoparticles. Journal Physics D: Applied Physics, 2019, 52, 363002.	2.8	7
21	High-resolution tip-enhanced Raman scattering probes sub-molecular density changes. Nature Communications, 2019, 10, 2567.	12.8	51
22	Atomistic Characterization of Plasmonic Dimers in the Quantum Size Regime. Journal of Physical Chemistry C, 2019, 123, 13900-13907.	3.1	11
23	Doubly resonant sum frequency spectroscopy of mixed photochromic isomers on surfaces reveals conformation-specific vibronic effects. Journal of Chemical Physics, 2019, 150, 114704.	3.0	20
24	Non-Condon Effects in the Resonance Hyper-Raman Scattering of Chalcogen-Substituted Rhodamine Derivatives. Journal of Physical Chemistry C, 2018, 122, 25051-25058.	3.1	2
25	A Discrete Interaction Model/Quantum Mechanical Method for Simulating Plasmon-Enhanced Two-Photon Absorption. Journal of Chemical Theory and Computation, 2018, 14, 5896-5903.	5.3	9
26	Using SERS To Understand the Binding of N-Heterocyclic Carbenes to Gold Surfaces. Journal of Physical Chemistry Letters, 2018, 9, 6779-6785.	4.6	38
27	Morphology dependent near-field response in atomistic plasmonic nanocavities. Nanoscale, 2018, 10, 11410-11417.	5.6	34
28	Microscopy with a single-molecule scanning electrometer. Science Advances, 2018, 4, eaat5472.	10.3	40
29	Comparison of thermally actuated retro-diels-alder release groups for nanoparticle based nucleic acid delivery. Journal of Colloid and Interface Science, 2018, 526, 312-321.	9.4	19
30	Surface-Enhanced Resonance Hyper-Raman Scattering Elucidates the Molecular Orientation of Rhodamine 6G on Silver Colloids. Journal of Physical Chemistry Letters, 2017, 8, 1819-1823.	4.6	30
31	Importance of double-resonance effects in two-photon absorption properties of Au₂₅(SR)₁₈^{â°'}. Chemical Science, 2017, 8, 4595-4601.	7.4	14
32	Single-Molecule Imaging Using Atomistic Near-Field Tip-Enhanced Raman Spectroscopy. ACS Nano, 2017, 11, 5094-5102.	14.6	92
33	Quantum Mechanical Calculations of Vibrational Sum-Frequency-Generation (SFG) Spectra of Cellulose: Dependence of the CH and OH Peak Intensity on the Polarity of Cellulose Chains within the SFG Coherence Domain. Journal of Physical Chemistry Letters, 2017, 8, 55-60.	4.6	28
34	Tip-Enhanced Raman Voltammetry: Coverage Dependence and Quantitative Modeling. Nano Letters, 2017, 17, 590-596.	9.1	74
35	Tip-Enhanced Raman Spectromicroscopy of Co(II)-Tetraphenylporphyrin on Au(111): Toward the Chemistsâ€™ Microscope. ACS Nano, 2017, 11, 11466-11474.	14.6	63
36	Enhanced detection of explosives by turn-on resonance Raman upon hostâ€“guest complexation in solution and the solid state. Chemical Communications, 2017, 53, 10918-10921.	4.1	9

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37	Experimental and Theoretical Study of Azimuth Angle and Polarization Dependences of Sum-Frequency-Generation Vibrational Spectral Features of Uniaxially Aligned Cellulose Crystals. Journal of Physical Chemistry C, 2017, 121, 18876-18886.	3.1	21
38	External orthogonality in subsystem time-dependent density functional theory. Physical Chemistry Chemical Physics, 2016, 18, 21032-21039.	2.8	33
39	Theory of Linear and Nonlinear Surface-Enhanced Vibrational Spectroscopies. Annual Review of Physical Chemistry, 2016, 67, 541-564.	10.8	44
40	Simulating Ensemble-Averaged Surface-Enhanced Raman Scattering. Journal of Physical Chemistry C, 2016, 120, 20833-20842.	3.1	26
41	Chain Length and Solvent Control over the Electronic Properties of Alkanethiolate-Protected Gold Nanoparticles at the Molecule-to-Metal Transition. Journal of the American Chemical Society, 2016, 138, 15987-15993.	13.7	27
42	Toward Monitoring Electrochemical Reactions with Dual-Wavelength SERS: Characterization of Rhodamine 6G (R6G) Neutral Radical Species and Covalent Tethering of R6G to Silver Nanoparticles. Journal of Physical Chemistry C, 2016, 120, 24982-24991.	3.1	52
43	Simulating Surface-Enhanced Hyper-Raman Scattering Using Atomistic Electrodynamics-Quantum Mechanical Models. Journal of Chemical Theory and Computation, 2016, 12, 5968-5978.	5.3	19
44	Conformational Contrast of Surface-Mediated Molecular Switches Yields Ã...ngstrom-Scale Spatial Resolution in Ultrahigh Vacuum Tip-Enhanced Raman Spectroscopy. Nano Letters, 2016, 16, 7774-7778.	9.1	96
45	Understanding the shape effect on the plasmonic response of small ligand coated nanoparticles. Journal of Optics (United Kingdom), 2016, 18, 074009.	2.2	25
46	Probing Two-Photon Molecular Properties with Surface-Enhanced Hyper-Raman Scattering: A Combined Experimental and Theoretical Study of Crystal Violet. Journal of Physical Chemistry C, 2016, 120, 20936-20942.	3.1	13
47	Simulating Third-Order Nonlinear Optical Properties Using Damped Cubic Response Theory within Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2016, 12, 1294-1304.	5.3	19
48	Orbital Renormalization Effects on the Coupling between Molecular Excitations and Plasmons. Journal of Physical Chemistry C, 2016, 120, 5659-5666.	3.1	6
49	Atomistic electrodynamics simulations of bare and ligand-coated nanoparticles in the quantum size regime. Nature Communications, 2015, 6, 8921.	12.8	69
50	Influence of shape on the optical properties of hematite aerosol. Journal of Geophysical Research D: Atmospheres, 2015, 120, 7025-7039.	3.3	17
51	Hydroxyl and amino functionalized cyclometalated Ir(III) complexes: Synthesis, characterization and cytotoxicity studies. Journal of Organometallic Chemistry, 2015, 791, 175-182.	1.8	18
52	Plasmonic Circular Dichroism of 310- and Î±-Helix Using a Discrete Interaction Model/Quantum Mechanics Method. Journal of Physical Chemistry A, 2015, 119, 5218-5223.	2.5	12
53	Frozen Density Embedding with External Orthogonality in Delocalized Covalent Systems. Journal of Chemical Theory and Computation, 2015, 11, 3080-3088.	5.3	29
54	Understanding the Effect of Monomeric Iridium(III/IV) Aquo Complexes on the Photoelectrochemistry of IrO_xÂ·nH₂O-Catalyzed Water-Splitting Systems. Journal of the American Chemical Society, 2015, 137, 8749-8757.	13.7	41

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55	Molecular-Resolution Interrogation of a Porphyrin Monolayer by Ultrahigh Vacuum Tip-Enhanced Raman and Fluorescence Spectroscopy. Nano Letters, 2015, 15, 4114-4120.	9.1	86
56	Surface-Enhanced Spectroscopy for Higher-Order Light Scattering: A Combined Experimental and Theoretical Study of Second Hyper-Raman Scattering. Journal of Physical Chemistry Letters, 2015, 6, 5067-5071.	4.6	19
57	Simulation of resonance hyper-Rayleigh scattering of molecules and metal clusters using a time-dependent density functional theory approach. Journal of Chemical Physics, 2014, 141, 124305.	3.0	21
58	A Hybrid Atomistic Electrodynamicsâ€“Quantum Mechanical Approach for Simulating Surface-Enhanced Raman Scattering. Accounts of Chemical Research, 2014, 47, 88-99.	15.6	91
59	Intramolecular Insight into Adsorbateâ€“Substrate Interactions via Low-Temperature, Ultrahigh-Vacuum Tip-Enhanced Raman Spectroscopy. Journal of the American Chemical Society, 2014, 136, 3881-3887.	13.7	123
60	Simulating Surface-Enhanced Raman Optical Activity Using Atomistic Electrodynamics-Quantum Mechanical Models. Journal of Physical Chemistry A, 2014, 118, 9069-9079.	2.5	24
61	Non-Condon Effects on the Doubly Resonant Sum Frequency Generation of Rhodamine 6G. Journal of Physical Chemistry Letters, 2014, 5, 329-335.	4.6	22
62	Investigation of Linear and Nonlinear Raman Scattering for Isotopologues of Ru(bpy)₃²⁺. Journal of Physical Chemistry C, 2013, 117, 20855-20866.	3.1	17
63	Determining Molecular Orientation With Surface-Enhanced Raman Scattering Using Inhomogenous Electric Fields. Journal of Physical Chemistry C, 2013, 117, 19622-19631.	3.1	74
64	Tuning surface-enhanced Raman scattering from graphene substrates using the electric field effect and chemical doping. Applied Physics Letters, 2013, 102, 11102.	3.3	48
65	Quantum Size Effects in the Optical Properties of Ligand Stabilized Aluminum Nanoclusters. Journal of Physical Chemistry C, 2013, 117, 6741-6746.	3.1	20
66	Surface-Enhanced Hyper-Raman Scattering Elucidates the Two-Photon Absorption Spectrum of Rhodamine 6G. Journal of Physical Chemistry C, 2013, 117, 3046-3054.	3.1	35
67	Direct Test of the Equivalency of Dynamic IR and Dynamic Raman Spectroscopies As Techniques for Observing Ultrafast Molecular Dynamics. Journal of Physical Chemistry A, 2013, 117, 2067-2074.	2.5	9
68	Photoreaction of Matrix-Isolated Dihydroazulene-Functionalized Molecules on Au{111}. Nano Letters, 2013, 13, 337-343.	9.1	21
69	A discrete interaction model/quantum mechanical method for simulating nonlinear optical properties of molecules near metal surfaces. Molecular Physics, 2013, 111, 1322-1331.	1.7	12
70	The Origin of Relative Intensity Fluctuations in Single-Molecule Tip-Enhanced Raman Spectroscopy. Journal of the American Chemical Society, 2013, 135, 17187-17192.	13.7	96
71	Simulating One-Photon Absorption and Resonance Raman Scattering Spectra Using Analytical Excited State Energy Gradients within Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2013, 9, 5490-5503.	5.3	49
72	Vibronic coupling simulations for linear and nonlinear optical processes: Simulation results. Journal of Chemical Physics, 2012, 136, 064110.	3.0	32

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73	Vibronic coupling simulations for linear and nonlinear optical processes: Theory. Journal of Chemical Physics, 2012, 136, 064111.	3.0	73
74	Effect of Tether Conductivity on the Efficiency of Photoisomerization of Azobenzene-Functionalized Molecules on Au{111}. Journal of Physical Chemistry Letters, 2012, 3, 2388-2394.	4.6	23
75	Importance of Correctly Describing Charge-Transfer Excitations for Understanding the Chemical Effect in SERS. Journal of Physical Chemistry Letters, 2012, 3, 2470-2475.	4.6	85
76	Surface-Enhanced Raman Spectroscopy To Probe Photoreaction Pathways and Kinetics of Isolated Reactants on Surfaces: Flat versus Curved Substrates. Nano Letters, 2012, 12, 5362-5368.	9.1	40
77	Surface-Enhanced Raman Scattering Study on Graphene-Coated Metallic Nanostructure Substrates. Journal of Physical Chemistry C, 2012, 116, 7249-7254.	3.1	97
78	A discrete interaction model/quantum mechanical method for simulating surface-enhanced Raman spectroscopy. Journal of Chemical Physics, 2012, 136, 214103.	3.0	60
79	Single-Molecule Tip-Enhanced Raman Spectroscopy. Journal of Physical Chemistry C, 2012, 116, 478-483.	3.1	226
80	On the chemical enhancement in SERS. AIP Conference Proceedings, 2012, , .	0.4	1
81	Metallic Membranes with Subwavelength Complementary Patterns: Distinct Substrates for Surface-Enhanced Raman Scattering. ACS Nano, 2011, 5, 5472-5477.	14.6	17
82	Scalable Manufacturing of Plasmonic Nanodisk Dimers and Cusp Nanostructures Using Salting-out Quenching Method and Colloidal Lithography. ACS Nano, 2011, 5, 5838-5847.	14.6	28
83	A discrete interaction model/quantum mechanical method to describe the interaction of metal nanoparticles and molecular absorption. Journal of Chemical Physics, 2011, 135, 134103.	3.0	76
84	Probing Two-Photon Properties of Molecules: Large Non-Condon Effects Dominate the Resonance Hyper-Raman Scattering of Rhodamine 6G. Journal of the American Chemical Society, 2011, 133, 14590-14592.	13.7	40
85	Theoretical Studies of Plasmonics using Electronic Structure Methods. Chemical Reviews, 2011, 111, 3962-3994.	47.7	393
86	Surface-Enhanced Raman Spectroscopy to Probe Reversibly Photoswitchable Azobenzene in Controlled Nanoscale Environments. Nano Letters, 2011, 11, 3447-3452.	9.1	100
87	Molecular Logic Gates Using Surface-Enhanced Raman-Scattered Light. Journal of the American Chemical Society, 2011, 133, 7288-7291.	13.7	43
88	Probing Oneâ€Photon Inaccessible Electronic States with High Sensitivity: Wavelength Scanned Surface Enhanced Hyperâ€Raman Scattering. ChemPhysChem, 2011, 12, 101-103.	2.1	23
89	Dynamic Tuning of Plasmonâ€“Exciton Coupling in Arrays of Nanodiskâ€“Jâ€aggregate Complexes. Advanced Materials, 2010, 22, 3603-3607.	21.0	80
90	Theoretical studies of surface enhanced hyper-Raman spectroscopy: The chemical enhancement mechanism. Journal of Chemical Physics, 2010, 133, 054103.	3.0	45

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91	A discrete interaction model/quantum mechanical method for describing response properties of molecules adsorbed on metal nanoparticles. Journal of Chemical Physics, 2010, 133, 074103.	3.0	87
92	Assessment of the accuracy of long-range corrected functionals for describing the electronic and optical properties of silver clusters. Journal of Chemical Physics, 2010, 132, 194302.	3.0	49
93	Auâ^'Cu Alloy Nanoparticles with Tunable Compositions and Plasmonic Properties: Experimental Determination of Composition and Correlation with Theory. Journal of Physical Chemistry C, 2010, 114, 19263-19269.	3.1	165
94	Understanding the Resonance Raman Scattering of Donorâ^'Acceptor Complexes using Long-Range Corrected DFT. Journal of Chemical Theory and Computation, 2010, 6, 2845-2855.	5.3	23
95	Effects of Intrinsic Fano Interference on Surface Enhanced Raman Spectroscopy: Comparison between Platinum and Gold. Journal of Physical Chemistry C, 2010, 114, 18059-18066.	3.1	46
96	Calculation of Absolute Resonance Raman Intensities: Vibronic Theory vs Short-Time Approximation. Journal of Physical Chemistry C, 2010, 114, 5540-5546.	3.1	47
97	Turning on Resonant SERRS Using the Chromophoreâ^'Plasmon Coupling Created by Hostâ^'Guest Complexation at a Plasmonic Nanoarray. Journal of the American Chemical Society, 2010, 132, 6099-6107.	13.7	44
98	Nonmetallic electronegativity equalization and point-dipole interaction model including exchange interactions for molecular dipole moments and polarizabilities. Journal of Chemical Physics, 2009, 131, 044101.	3.0	28
99	Surface-Enhanced Vibrational Raman Optical Activity: A Time-Dependent Density Functional Theory Approach. Journal of Physical Chemistry A, 2009, 113, 4437-4444.	2.5	31
100	Dynamic Control of Plasmon-Exciton Coupling in Au Nanodiskâ€"J-Aggregate Hybrid Nanostructure Arrays. Materials Research Society Symposia Proceedings, 2009, 1208, 1.	0.1	0
101	Reply to â€œComment on â€˜Excited States of DNA Base Pairs Using Long-Range Corrected Time-Dependent Density Functional Theoryâ€™â€• Journal of Physical Chemistry A, 2009, 113, 11095-11095.	2.5	3
102	Excited States of DNA Base Pairs Using Long-Range Corrected Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 9761-9765.	2.5	64
103	Atomistic Electrodynamics Model for Optical Properties of Silver Nanoclusters. Journal of Physical Chemistry C, 2009, 113, 15182-15190.	3.1	77
104	Determination of Binding Strengths of a Hostâ^'Guest Complex Using Resonance Raman Scattering. Journal of Physical Chemistry A, 2009, 113, 9450-9457.	2.5	31
105	Chemically Tuning the Localized Surface Plasmon Resonances of Gold Nanostructure Arrays. Journal of Physical Chemistry C, 2009, 113, 7019-7024.	3.1	63
106	Excitation Energies of Zinc Porphyrin in Aqueous Solution Using Long-Range Corrected Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 6041-6043.	2.5	60
107	Active Molecular Plasmonics: Controlling Plasmon Resonances with Molecular Switches. Nano Letters, 2009, 9, 819-825.	9.1	213
108	Understanding the Moleculeâ^'Surface Chemical Coupling in SERS. Journal of the American Chemical Society, 2009, 131, 4090-4098.	13.7	371

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109	Coupling between Molecular and Plasmonic Resonances: Effect of Molecular Absorbance. Journal of Physical Chemistry C, 2009, 113, 18499-18503.	3.1	51
110	Controlling the non-resonant chemical mechanism of SERS using a molecular photoswitch. Physical Chemistry Chemical Physics, 2009, 11, 7424.	2.8	24
111	Electronic structure methods for studying surface-enhanced Raman scattering. Chemical Society Reviews, 2008, 37, 1061.	38.1	568
112	Effects of Geometry and Composition on Charge-Induced Plasmonic Shifts in Gold Nanoparticles. Journal of Physical Chemistry C, 2008, 112, 7309-7317.	3.1	79
113	Electrostatic Interaction Model for the Calculation of the Polarizability of Large Noble Metal Nanoclusters. Journal of Physical Chemistry C, 2008, 112, 15697-15703.	3.1	75
114	Resonance vibrational Raman optical activity: A time-dependent density functional theory approach. Journal of Chemical Physics, 2007, 127, 134101.	3.0	78
115	Size-Dependence of the Enhanced Raman Scattering of Pyridine Adsorbed on Agn(n= 2â^'8, 20) Clusters. Journal of Physical Chemistry C, 2007, 111, 4756-4764.	3.1	180
116	Microscopic polarization in ropes and films of aligned carbon nanotubes. Journal of Computational Methods in Sciences and Engineering, 2007, 6, 353-364.	0.2	1
117	Interaction of Plasmon and Molecular Resonances for Rhodamine 6G Adsorbed on Silver Nanoparticles. Journal of the American Chemical Society, 2007, 129, 7647-7656.	13.7	282
118	Surface-Enhanced Raman Scattering of Pyrazine at the Junction between Two Ag20Nanoclusters. Nano Letters, 2006, 6, 1229-1234.	9.1	212
119	Resonance Raman Scattering of Rhodamine 6G as Calculated Using Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2006, 110, 5973-5977.	2.5	344
120	Pyridineâ^'Ag20 Cluster:â€‰ A Model System for Studying Surface-Enhanced Raman Scattering. Journal of the American Chemical Society, 2006, 128, 2911-2919.	13.7	478
121	Coupled Cluster and Density Functional Theory Studies of the Vibrational Contribution to the Optical Rotation of (S)-Propylene Oxide. Journal of the American Chemical Society, 2006, 128, 976-982.	13.7	77
122	THE DISCRETE SOLVENT REACTION FIELD MODEL: A QUANTUM MECHANICS/MOLECULAR MECHANICS MODEL FOR CALCULATING NONLINEAR OPTICAL PROPERTIES OF MOLECULES IN CONDENSED PHASE. , 2006, , 283-325.		3
123	Time-Dependent Density Functional Calculations of Optical Rotatory Dispersion Including Resonance Wavelengths as a Potentially Useful Tool for Determining Absolute Configurations of Chiral Molecules. Journal of Physical Chemistry A, 2006, 110, 2461-2473.	2.5	72
124	Circular dichroism spectrum of [Co(en)3]3+in water: A discrete solvent reaction field study. International Journal of Quantum Chemistry, 2006, 106, 2479-2488.	2.0	30
125	Refractive index and third-order nonlinear susceptibility of C60 in the condensed phase calculated with the discrete solvent reaction field model. International Journal of Quantum Chemistry, 2005, 102, 612-619.	2.0	22
126	Theory and method for calculating resonance Raman scattering from resonance polarizability derivatives. Journal of Chemical Physics, 2005, 123, 174110.	3.0	169

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127	Microscopic and macroscopic polarization within a combined quantum mechanics and molecular mechanics model. Journal of Chemical Physics, 2005, 122, 034103.	3.0	39
128	The first hyperpolarizability of p-nitroaniline in 1,4-dioxane: A quantum mechanical/molecular mechanics study. Journal of Chemical Physics, 2005, 123, 074307.	3.0	68
129	Frequency-Dependent Polarizabilities of Amino Acids as Calculated by an Electrostatic Interaction Model. Journal of Chemical Theory and Computation, 2005, 1, 626-633.	5.3	20
130	Finite lifetime effects on the polarizability within time-dependent density-functional theory. Journal of Chemical Physics, 2005, 122, 224115.	3.0	161
131	Size-scaling of the polarizability of tubular fullerenes investigated with time-dependent (current)-density-functional theory. Chemical Physics Letters, 2004, 395, 274-278.	2.6	30
132	The Static Polarizability and Second Hyperpolarizability of Fullerenes and Carbon Nanotubesâ€. Journal of Physical Chemistry A, 2004, 108, 8795-8800.	2.5	41
133	Microscopic and Macroscopic Polarization in C60 Fullerene Clusters as Calculated by an Electrostatic Interaction Model. Journal of Physical Chemistry B, 2004, 108, 8226-8233.	2.6	31
134	A discrete solvent reaction field model within density functional theory. Journal of Chemical Physics, 2003, 118, 514-521.	3.0	98
135	Saturation of the Third-Order Polarizability of Carbon Nanotubes Characterized by a Dipole Interaction Model. Nano Letters, 2003, 3, 661-665.	9.1	32
136	A Dipole Interaction Model for the Molecular Second Hyperpolarizability. Journal of Physical Chemistry A, 2003, 107, 2270-2276.	2.5	43
137	A discrete solvent reaction field model for calculating molecular linear response properties in solution. Journal of Chemical Physics, 2003, 119, 3800-3809.	3.0	76
138	A discrete solvent reaction field model for calculating frequency-dependent hyperpolarizabilities of molecules in solution. Journal of Chemical Physics, 2003, 119, 12998-13006.	3.0	47
139	Collision effects in the nonlinear Raman response of liquid carbon disulfide. Journal of Chemical Physics, 2002, 116, 3277-3285.	3.0	26
140	Medium perturbations on the molecular polarizability calculated within a localized dipole interaction model. Journal of Chemical Physics, 2002, 117, 3316-3320.	3.0	36
141	Polarizability of molecular clusters as calculated by a dipole interaction model. Journal of Chemical Physics, 2002, 116, 4001-4010.	3.0	180
142	Frequency-Dependent Polarizability of Boron Nitride Nanotubes:Â A Theoretical Study. Journal of Physical Chemistry B, 2001, 105, 10243-10248.	2.6	42
143	An atomic capacitance-polarizability model for the calculation of molecular dipole moments and polarizabilities. International Journal of Quantum Chemistry, 2001, 84, 513-522.	2.0	34
144	Static and Frequency-Dependent Polarizability Tensors for Carbon Nanotubes. Journal of Physical Chemistry B, 2000, 104, 10462-10466.	2.6	64

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145	Frequency-Dependent Molecular Polarizability Calculated within an Interaction Model. Journal of Physical Chemistry A, 2000, 104, 1563-1569.	2.5	60