Rebecca L Gieseking

List of Publications by Year
in descending order

31 papers	1,043 citations	471509 17 h-index	454955 30 g-index
35 all docs	35 docs citations	35 times ranked	1596 citing authors

#	Article	IF	Citations
1	Plasmons: untangling the classical, experimental, and quantum mechanical definitions. Materials Horizons, 2022, 9, 25-42.	12.2	13
2	Evolution of plasmon-like excited states in silver nanowires and nanorods. Journal of Chemical Physics, 2022, 156, 074301.	3.0	5
3	Quantum Mechanical Effects in High-Resolution Tip-Enhanced Raman Imaging. Journal of Physical Chemistry C, 2022, 126, 11690-11700.	3.1	2
4	A new release of <scp>MOPAC</scp> incorporating the <scp>INDO</scp>/S semiempirical model with <scp>CI</scp> excited states. Journal of Computational Chemistry, 2021, 42, 365-378.	3.3	18
5	Hydride- and halide-substituted Au₉(PH₃)₈³⁺ nanoclusters: similar absorption spectra disguise distinct geometries and electronic structures. Physical Chemistry Chemical Physics, 2021, 23, 17287-17299.	2.8	4
6	Horizons Community Board collection: solar energy conversion. Nanoscale Horizons, 2021, 6, 839-841.	8.0	0
7	Analytical Approaches To Identify Plasmon-like Excited States in Bare and Ligand-Protected Metal Nanoclusters. Journal of Physical Chemistry C, 2020, 124, 3260-3269.	3.1	19
8	Third-Order Nonlinear Optical Properties of Ag Nanoclusters: Connecting Molecule-like and Nanoparticle-like Behavior. Chemistry of Materials, 2019, 31, 6850-6859.	6.7	23
9	Molecular engineering of organic semiconductors enables noble metal-comparable SERS enhancement and sensitivity. Nature Communications, 2019, 10, 5502.	12.8	84
10	Bias-Dependent Chemical Enhancement and Nonclassical Stark Effect in Tip-Enhanced Raman Spectromicroscopy of CO-Terminated Ag Tips. Journal of Physical Chemistry Letters, 2018, 9, 3074-3080.	4.6	32
11	Benchmarking Semiempirical Methods To Compute Electrochemical Formal Potentials. Journal of Physical Chemistry A, 2018, 122, 6809-6818.	2.5	15
12	Theoretical modeling of voltage effects and the chemical mechanism in surface-enhanced Raman scattering. Faraday Discussions, 2017, 205, 149-171.	3.2	40
13	Assessment of Front-Substituted Zwitterionic Cyanine Polymethines for All-Optical Switching Applications. Journal of Physical Chemistry C, 2017, 121, 14166-14175.	3.1	10
14	Semiempirical modeling of electrochemical charge transfer. Faraday Discussions, 2017, 199, 547-563.	3.2	17
15	Nanostructured organic semiconductor films for molecular detection with surface-enhanced Raman spectroscopy. Nature Materials, 2017, 16, 918-924.	27.5	229
16	Quantum Mechanical Identification of Quadrupolar Plasmonic Excited States in Silver Nanorods. Journal of Physical Chemistry A, 2016, 120, 9324-9329.	2.5	17
17	Implementation of INDO/SCI with COSMO Implicit Solvation and Benchmarking for Solvatochromic Shifts. Journal of Physical Chemistry A, 2016, 120, 9878-9885.	2.5	6
18	Review of Plasmon-Induced Hot-Electron Dynamics and Related SERS Chemical Effects. ACS Symposium Series, 2016, , 1-22.	0.5	19

#	Article	IF	Citations
19	Benchmarking Density Functional Theory Approaches for the Description of Symmetry Breaking in Long Polymethine Dyes. Journal of Physical Chemistry C, 2016, 120, 9975-9984.	3.1	25
20	Benchmarking Post-Hartreeâ€“Fock Methods To Describe the Nonlinear Optical Properties of Polymethines: An Investigation of the Accuracy of Algebraic Diagrammatic Construction (ADC) Approaches. Journal of Chemical Theory and Computation, 2016, 12, 5465-5476.	5.3	13
21	Understanding the Relationships Among Molecular Structure, Excited-State Properties, and Polarizabilities of Ï€-Conjugated Chromophores. Materials and Energy, 2016, , 393-419.	0.1	1
22	Semiempirical Modeling of Ag Nanoclusters: New Parameters for Optical Property Studies Enable Determination of Double Excitation Contributions to Plasmonic Excitation. Journal of Physical Chemistry A, 2016, 120, 4542-4549.	2.5	45
23	Recognition of halides and Y-shaped oxoanions by carbonylchromium-based urea-like molecules: A theoretical analysis of hydrogen bonding modes. Journal of Molecular Graphics and Modelling, 2016, 64, 1-10.	2.4	3
24	Distinguishing the Effects of Bond-Length Alternation versus Bond-Order Alternation on the Nonlinear Optical Properties of Ï€-Conjugated Chromophores. Journal of Physical Chemistry Letters, 2015, 6, 2158-2162.	4.6	75
25	Nonlinear Optical Properties of X(C₆H₅)₄ (X = B^{â€“}, C,) Tj ETQq1 1 0.784314 rgBT Journal of the American Chemical Society, 2015, 137, 9635-9642.	13.7	21
26	25th Anniversary Article: Design of Polymethine Dyes for Allâ€Optical Switching Applications: Guidance from Theoretical and Computational Studies. Advanced Materials, 2014, 26, 68-84.	21.0	97
27	Effect of Bulky Substituents on Thiopyrylium Polymethine Aggregation in the Solid State: A Theoretical Evaluation of the Implications for All-Optical Switching Applications. Chemistry of Materials, 2014, 26, 6439-6447.	6.7	18
28	Impact of the Nature of the Excited-State Transition Dipole Moments on the Third-Order Nonlinear Optical Response of Polymethine Dyes for All-Optical Switching Applications. ACS Photonics, 2014, 1, 261-269.	6.6	35
29	Polymethine materials with solid-state third-order optical susceptibilities suitable for all-optical signal-processing applications. Materials Horizons, 2014, 1, 577-581.	12.2	59
30	Impact of Bulk Aggregation on the Electronic Structure of Streptocyanines: Implications for the Solid-State Nonlinear Optical Properties and All-Optical Switching Applications. Journal of Physical Chemistry C, 2014, 118, 23575-23585.	3.1	20
31	Complementary halogen and hydrogen bonding: sulfurâ‹¯iodine interactions and thioamide ribbons. Chemical Communications, 2010, 46, 1854-1856.	4.1	78