Paul N Day

List of Publications by Year
in descending order

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20 papers	615 citations	759055 12 h-index	752573 20 g-index
20 all docs	20 docs citations	20 times ranked	829 citing authors

#	Article	IF	Citations
1	Understanding Structural and Optical Properties of Nanoscale CdSe Magic-Size Quantum Dots: Insight from Computational Prediction. Journal of Physical Chemistry C, 2010, 114, 16197-16209.	1.5	115
2	TDDFT Study of One- and Two-Photon Absorption Properties:Â Donorâ^'Ï€â^'Acceptor Chromophores. Journal of Physical Chemistry B, 2005, 109, 1803-1814.	1.2	101
3	Calculation of two-photon absorption spectra of donor-Ï€-acceptor compounds in solution using quadratic response time-dependent density functional theory. Journal of Chemical Physics, 2006, 125, 094103.	1.2	63
4	Computational Prediction of Structures and Optical Excitations for Nanoscale Ultrasmall ZnS and CdSe Clusters. Journal of Chemical Theory and Computation, 2013, 9, 3581-3596.	2.3	51
5	Calculation of One- and Two-Photon Absorption Spectra of Thiolated Gold Nanoclusters using Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2010, 6, 2809-2821.	2.3	47
6	The performance and relationship among range-separated schemes for density functional theory. Journal of Chemical Physics, 2011, 135, 074109.	1.2	43
7	Linear and Nonlinear Optical Response in Silver Nanoclusters: Insight from a Computational Investigation. Journal of Physical Chemistry A, 2016, 120, 507-518.	1.1	31
8	One- and Two-Photon Spectra of Platinum Acetylide Chromophores: A TDDFT Study. Journal of Physical Chemistry A, 2009, 113, 13943-13952.	1.1	28
9	Calculation of One-Photon and Two-Photon Absorption Spectra of Porphyrins Using Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2008, 4, 1094-1106.	2.3	27
10	Analytical energy gradients of Coulombâ€attenuated timeâ€dependent density functional methods for excited states. International Journal of Quantum Chemistry, 2010, 110, 2247-2255.	1.0	22
11	Effects of conjugation in length and dimension on two-photon properties of fluorene-based chromophores. Theoretical Chemistry Accounts, 2008, 120, 167-175.	0.5	19
12	Theoretical analysis of structures and electronic spectra in molecular cadmium chalcogenide clusters. Journal of Chemical Physics, 2015, 142, 234305.	1.2	18
13	Systematic Study of Structure, Stability, and Electronic Absorption of Tetrahedral CdSe Clusters with Carboxylate and Amine Ligands. Journal of Physical Chemistry A, 2018, 122, 6704-6712.	1.1	10
14	Theoretical Prediction of Optical Absorption and Emission in Thiolated Gold Clusters. Journal of Physical Chemistry A, 2019, 123, 6472-6481.	1.1	9
15	Systematic Study of the Properties of CdS Clusters with Carboxylate Ligands Using a Deep Neural Network Potential Developed with Data from Density Functional Theory Calculations. Journal of Physical Chemistry A, 2020, 124, 10472-10481.	1.1	9
16	A Theoretical Investigation of the Structure and Optical Properties of a Silver Cluster in Solid Form and in Solution. Journal of Physical Chemistry A, 2017, 121, 326-333.	1.1	7
17	Calculations of One- and Two-Photon Absorption Spectra for Molecular Metal Chalcogenide Clusters with Electron-Acceptor Ligands. Journal of Physical Chemistry A, 2017, 121, 1748-1759.	1.1	5
18	Theoretical Analysis of Optical Absorption and Emission in Mixed Noble Metal Nanoclusters. Journal of Physical Chemistry A, 2018, 122, 4058-4066.	1.1	5

#	Article	IF	Citations
19	Theoretical analysis of structures and electronic spectra of molecular colloidal cadmium sulfide clusters and nanoplatelets. Journal of Chemical Physics, 2021, 155, 094302.	1.2	4
20	Calculated linear and nonlinear optical absorption spectra of phosphine-ligated gold clusters. Physical Chemistry Chemical Physics, 2022, 24, 11234-11248.	1.3	1