Marco Caricato

List of Publications by Year
in descending order

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67	2,252	318942	252626
papers	citations	23 h-index	46 g-index

78	78	78	2564
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Basis Set Dependence of Optical Rotation Calculations with Different Choices of Gauge. Journal of Physical Chemistry A, 2022, 126, 1861-1870.	1.1	5
2	Origin invariant electronic circular dichroism in the length dipole gauge without London atomic orbitals. Journal of Chemical Physics, 2022, 156, 154114.	1.2	7
3	Full optical rotation tensor at coupled cluster with single and double excitations level in the modified velocity gauge. Chirality, 2021, 33, 303-314.	1.3	11
4	Gauge Dependence of the Sl*f* Molecular Orbital Space Decomposition of Optical Rotation. Journal of Physical Chemistry A, 2021, 125, 4976-4985.	1.1	4
5	Origin invariant full optical rotation tensor in the length dipole gauge without London atomic orbitals. Journal of Chemical Physics, 2021, 155, 024118.	1.2	11
6	Predicted Properties of Active Catalyst Sites on Amorphous Silica: Impact of Silica Preoptimization Protocol. Industrial & Engineering Chemistry Research, 2021, 60, 12834-12846.	1.8	11
7	Cluster Model Simulations of Metal-Doped Amorphous Silicates for Heterogeneous Catalysis. Journal of Physical Chemistry C, 2021, 125, 27509-27519.	1.5	8
8	A molecular orbital selection approach for fast calculations of specific rotation with density functional theory. Chirality, 2020, 32, 243-253.	1.3	3
9	Benchmark Study of Ground-State Raman Spectra in Conjugated Molecules. Journal of Chemical Theory and Computation, 2020, 16, 612-620.	2.3	6
10	Origin invariant optical rotation in the length dipole gauge without London atomic orbitals. Journal of Chemical Physics, 2020, 153, 151101.	1.2	17
11	On the Discrepancy between Experimental and Calculated Raman Intensities for Conjugated Phenyl and Thiophene Derivatives. Journal of Physical Chemistry A, 2020, 124, 4678-4689.	1.1	7
12	Multistate QM/QM Extrapolation of UV/Vis Absorption Spectra with Point Charge Embedding. Journal of Chemical Theory and Computation, 2020, 16, 4361-4372.	2.3	12
13	Compact Basis Sets for Optical Rotation Calculations. Journal of Chemical Theory and Computation, 2020, 16, 4408-4415.	2.3	13
14	Surface Acidity Characterization of Metal-Doped Amorphous Silicates via Py-FTIR and ¹⁵N NMR Simulations. Journal of Physical Chemistry C, 2020, 124, 15231-15240.	1.5	20
15	Coupled cluster theory in the condensed phase within the singlesâ€T density scheme for the environment response. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1463.	6.2	6
16	Enhanced Olefin Metathesis Performance of Tungsten and Niobium Incorporated Bimetallic Silicates: Evidence of Synergistic Effects. ChemCatChem, 2020, 12, 2004-2013.	1.8	9
17	Femtosecond Stimulated Raman Scattering from Triplet Electronic States: Experimental and Theoretical Study of Resonance Enhancements. Journal of Physical Chemistry A, 2019, 123, 7720-7732.	1.1	9
18	Coupled Cluster Theory with Induced Dipole Polarizable Embedding for Ground and Excited States. Journal of Chemical Theory and Computation, 2019, 15, 4485-4496.	2.3	13

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19	Silica Supported Molecular Palladium Catalyst for Selective Hydrodeoxygenation of Aromatic Compounds under Mild Conditions. ACS Catalysis, 2019, 9, 9060-9071.	5.5	15
20	CCSDâ€PCM Excited State Energy Gradients with the Linear Response Singles Approximation to Study the Photochemistry of Molecules in Solution. ChemPhotoChem, 2019, 3, 747-754.	1.5	6
21	Configuration Space Analysis of the Specific Rotation of Helicenes. Journal of Physical Chemistry A, 2019, 123, 4406-4418.	1.1	9
22	Helical Chains of Diatomic Molecules as a Model for Solid-State Optical Rotation. Journal of Physical Chemistry C, 2019, 123, 4329-4340.	1.5	7
23	Coupled cluster theory with the polarizable continuum model of solvation. International Journal of Quantum Chemistry, 2019, 119, e25710.	1.0	18
24	Linear response coupled cluster theory with the polarizable continuum model within the singles approximation for the solvent response. Journal of Chemical Physics, 2018, 148, 134113.	1.2	8
25	Comparison of measured and predicted specific optical rotation in gas and solution phases: A test for the polarizable continuum model of solvation. Chirality, 2018, 30, 383-395.	1.3	17
26	A Benchmark Study of Electronic Couplings in Donorâ€“Bridgeâ€“Acceptor Systems with the FMR-B Method. Journal of Chemical Theory and Computation, 2018, 14, 2007-2016.	2.3	6
27	Catalytic Nâˆ’H Bond Activation and Breaking by a Wellâ€Đefined Co^{II}₁O₄ Site of a Heterogeneous Catalyst. ChemCatChem, 2018, 10, 736-742.	1.8	8
28	Computational Multinuclear NMR Characterization of Metal-Doped Amorphous Silica Catalysts. Chemistry of Materials, 2018, 30, 7813-7822.	3.2	10
29	Correlation of Active Site Precursors and Olefin Metathesis Activity in W-Incorporated Silicates. ACS Catalysis, 2018, 8, 10437-10445.	5.5	13
30	Probing Dynamics in Higher-Lying Electronic States with Resonance-Enhanced Femtosecond Stimulated Raman Spectroscopy. Journal of Physical Chemistry A, 2018, 122, 8308-8319.	1.1	23
31	How the Number of Layers and Relative Position Modulate the Interlayer Electron Transfer in Ï€-Stacked 2D Materials. Journal of Physical Chemistry Letters, 2017, 8, 1365-1370.	2.1	7
32	An EOM-CCSD-PCM Benchmark for Electronic Excitation Energies of Solvated Molecules. Journal of Chemical Theory and Computation, 2017, 13, 117-124.	2.3	22
33	Simulations of Ammonia Adsorption for the Characterization of Acid Sites in Metal-Doped Amorphous Silicates. Journal of Physical Chemistry C, 2017, 121, 22258-22267.	1.5	25
34	Electronic Coupling for Donor-Bridge-Acceptor Systems with a Bridge-Overlap Approach. Journal of Chemical Theory and Computation, 2017, 13, 4154-4161.	2.3	6
35	Triggering Emission with the Helical Turn in Thiadiazoleâ€Helicenes. Chemistry - A European Journal, 2017, 23, 437-446.	1.7	42
36	Accurate Assignments of Excited-State Resonance Raman Spectra: A Benchmark Study Combining Experiment and Theory. Journal of Physical Chemistry A, 2017, 121, 7937-7946.	1.1	26

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37	Point charge embedding for ONIOM excited states calculations. Journal of Chemical Physics, 2016, 145, 224109.	1.2	12
38	Multi-state extrapolation of UV/Vis absorption spectra with QM/QM hybrid methods. Journal of Chemical Physics, 2016, 144, 184102.	1.2	5
39	Evaluation of Electronic Coupling in Solids from Ab Initio Periodic Boundary Condition Calculations: The Case of Pentacene Crystal and Bilayer Graphene. Journal of Physical Chemistry C, 2016, 120, 17939-17948.	1.5	10
40	Conformational Effects on Specific Rotation: A Theoretical Study Based on the SÌƒk Method. Journal of Physical Chemistry A, 2015, 119, 8303-8310.	1.1	14
41	Orbital Analysis of Molecular Optical Activity Based on Configuration Rotatory Strength. Journal of Chemical Theory and Computation, 2015, 11, 1349-1353.	2.3	21
42	Electronic Couplings for Resonance Energy Transfer from CCSD Calculations: From Isolated to Solvated Systems. Journal of Chemical Theory and Computation, 2015, 11, 5219-5228.	2.3	12
43	Energy-Specific Equation-of-Motion Coupled-Cluster Methods for High-Energy Excited States: Application to K-edge X-ray Absorption Spectroscopy. Journal of Chemical Theory and Computation, 2015, 11, 4146-4153.	2.3	92
44	Assessment of low-scaling approximations to the equation of motion coupled-cluster singles and doubles equations. Journal of Chemical Physics, 2014, 141, 164116.	1.2	45
45	Large Solvation Effect in the Optical Rotatory Dispersion of Norbornenone. Angewandte Chemie - International Edition, 2014, 53, 1386-1389.	7.2	46
46	Insights on the Origin of the Unusually Large Specific Rotation of (1S,4S)-Norbornenone. Journal of Physical Chemistry A, 2014, 118, 4863-4871.	1.1	31
47	A corrected-linear response formalism for the calculation of electronic excitation energies of solvated molecules with the CCSD-PCM method. Computational and Theoretical Chemistry, 2014, 1040-1041, 99-105.	1.1	29
48	Implementation of the CCSD-PCM linear response function for frequency dependent properties in solution: Application to polarizability and specific rotation. Journal of Chemical Physics, 2013, 139, 114103.	1.2	29
49	A comparison between state-specific and linear-response formalisms for the calculation of vertical electronic transition energy in solution with the CCSD-PCM method. Journal of Chemical Physics, 2013, 139, 044116.	1.2	61
50	Vertical Electronic Excitations in Solution with the EOM-CCSD Method Combined with a Polarizable Explicit/Implicit Solvent Model. Journal of Chemical Theory and Computation, 2013, 9, 3035-3042.	2.3	48
51	Towards the Accurate and Efficient Calculation of Optical Rotatory Dispersion Using Augmented Minimal Basis Sets. Chirality, 2013, 25, 606-616.	1.3	26
52	Exploring Potential Energy Surfaces of Electronic Excited States in Solution with the EOM-CCSD-PCM Method. Journal of Chemical Theory and Computation, 2012, 8, 5081-5091.	2.3	50
53	Absorption and Emission Spectra of Solvated Molecules with the EOMâ€“CCSDâ€“PCM Method. Journal of Chemical Theory and Computation, 2012, 8, 4494-4502.	2.3	68
54	Oscillator Strengths in ONIOM Excited State Calculations. Journal of Chemical Theory and Computation, 2011, 7, 180-187.	2.3	10

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55	Oscillator Strength: How Does TDDFT Compare to EOM-CCSD?. Journal of Chemical Theory and Computation, 2011, 7, 456-466.	2.3	123
56	CCSD-PCM: Improving upon the reference reaction field approximation at no cost. Journal of Chemical Physics, 2011, 135, 074113.	1.2	42
57	Brueckner doubles coupled cluster method with the polarizable continuum model of solvation. Journal of Chemical Physics, 2011, 134, 244113.	1.2	19
58	Link atom bond length effect in ONIOM excited state calculations. Journal of Chemical Physics, 2010, 133, 054104.	1.2	10
59	Electronic excitation energies in solution at equation of motion CCSD level within a state specific polarizable continuum model approach. Journal of Chemical Physics, 2010, 132, 084102.	1.2	47
60	A variational formulation of the polarizable continuum model. Journal of Chemical Physics, 2010, 133, 014106.	1.2	125
61	A Comparison of Three Variants of the Generalized Davidson Algorithm for the Partial Diagonalization of Large Non-Hermitian Matrices. Journal of Chemical Theory and Computation, 2010, 6, 1966-1970.	2.3	16
62	Electronic Transition Energies: A Study of the Performance of a Large Range of Single Reference Density Functional and Wave Function Methods on Valence and Rydberg States Compared to Experiment. Journal of Chemical Theory and Computation, 2010, 6, 370-383.	2.3	202
63	Coupled Cluster Calculations in Solution with the Polarizable Continuum Model of Solvation. Journal of Physical Chemistry Letters, 2010, 1, 2369-2373.	2.1	41
64	On the difference between the transition properties calculated with linear response- and equation of motion-CCSD approaches. Journal of Chemical Physics, 2009, 131, 174104.	1.2	35
65	Using the ONIOM hybrid method to apply equation of motion CCSD to larger systems: Benchmarking and comparison with time-dependent density functional theory, configuration interaction singles, and time-dependent Hartreeâ€“Fock. Journal of Chemical Physics, 2009, 131, 134105.	1.2	15
66	Formation and relaxation of excited states in solution: A new time dependent polarizable continuum model based on time dependent density functional theory. Journal of Chemical Physics, 2006, 124, 124520.	1.2	484
67	Solvent polarity scales revisited: a ZINDO-PCM study of the solvatochromism of betaine-30. Molecular Physics, 2006, 104, 875-887.	0.8	43