Hrant P Hratchian

List of Publications by Year
in descending order

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59 papers	3,373 citations	257450 24 h-index	155660 55 g-index
88 all docs	88 docs citations	88 times ranked	3263 citing authors

#	Article	IF	Citations
1	A density functional theory investigation of the reaction of water with Ce2Oâ‚‚. Computational and Theoretical Chemistry, 2022, 1209, 113603.	2.5	0
2	Using projection operators with maximum overlap methods to simplify challenging selfâ€consistent field optimization. Journal of Computational Chemistry, 2022, 43, 382-390.	3.3	9
3	Comparison of Linear Response Theory, Projected Initial Maximum Overlap Method, and Molecular Dynamics-Based Vibronic Spectra: The Case of Methylene Blue. Journal of Chemical Theory and Computation, 2022, 18, 3039-3051.	5.3	2
4	Enhanced Reactivity for Aromatic Bromination via Halogen Bonding with Lactic Acid Derivatives. Journal of Organic Chemistry, 2022, 87, 8492-8502.	3.2	7
5	Photoelectron Spectra of Gd₂O₂^{â€“} and Nonmonotonic Photon-Energy-Dependent Variations in Populations of Close-Lying Neutral States. Journal of Physical Chemistry A, 2021, 125, 857-866.	2.5	9
6	Î”SCF Dyson orbitals and pole strengths from natural ionization orbitals. Journal of Chemical Physics, 2021, 154, 084104.	3.0	5
7	Versatile New Reagent for Nitrosation under Mild Conditions. Organic Letters, 2021, 23, 3253-3258.	4.6	8
8	Lanthanide Oxides: From Diatomics to High-Spin, Strongly Correlated Homo- and Heterometallic Clusters. Journal of Physical Chemistry A, 2021, 125, 6315-6331.	2.5	3
9	New Photoelectronâ€“Valence Electron Interactions Evident in the Photoelectron Spectrum of Gd₂O^{â€“}. Journal of Physical Chemistry A, 2021, 125, 9892-9903.	2.5	6
10	Assessing the Calculation of Exchange Coupling Constants and Spin Crossover Gaps Using the Approximate Projection Model To Improve Density Functional Calculations. Journal of Chemical Theory and Computation, 2020, 16, 154-163.	5.3	6
11	Unveiling the coexistence of cis- and trans-isomers in the hydrolysis of ZrO2: A coupled DFT and high-resolution photoelectron spectroscopy study. Journal of Chemical Physics, 2020, 153, 244308.	3.0	3
12	Exceptionally Complex Electronic Structures of Lanthanide Oxides and Small Molecules. Accounts of Chemical Research, 2019, 52, 3265-3273.	15.6	20
13	Experimental and Theoretical Evidence for Nitrogenâ€“Fluorine Halogen Bonding in Silver-Initiated Radical Fluorinations. ACS Catalysis, 2019, 9, 3322-3326.	11.2	29
14	Dispersion-Controlled Regioselective Acid-Catalyzed Intramolecular Hydroindolation of cis-Methindolylstyrenes To Access Tetrahydrobenzo[cd]indoles. Organic Letters, 2019, 21, 1574-1577.	4.6	10
15	Electronic and Molecular Structures of the CeB₆ Monomer. Journal of Physical Chemistry A, 2019, 123, 2040-2048.	2.5	22
16	Aiming toward an Effective Hispanic-Serving Chemistry Curriculum. ACS Symposium Series, 2019, , 49-66.	0.5	1
17	On the linear geometry of lanthanide hydroxide (Ln-OH, Ln = Laâ€“Lu). Physical Chemistry Chemical Physics, 2019, 21, 21890-21897.	2.8	1
18	On approximate projection models. Molecular Physics, 2019, 117, 1421-1429.	1.7	13

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19	High-resolution photoelectron spectroscopy of TiO3H2â^': Probing the TiO2â^' + H2O dissociative adduct. Journal of Chemical Physics, 2018, 148, 222810.	3.0	20
20	A Tale of Two Stabilities: How One Boron Atom Affects a Switch in Bonding Motifs in CeO₂B_x^{â€“} (x = 2, 3) Complexes. Journal of Physical Chemistry A, 2018, 122, 9879-9885.	2.5	9
21	Exotic electronic structures of SmxCe3â^'xOy (x = 0-3; y = 2-4) clusters and the effect of high neutral density of low-lying states on photodetachment transition intensities. Journal of Chemical Physics, 2018, 149, 054305.	3.0	13
22	Explaining the MoVO4â^' photoelectron spectrum: Rationalization of geometric and electronic structure. Journal of Chemical Physics, 2017, 146, 104301.	3.0	14
23	Modeling emission features of salicylidene aniline molecular crystals: A QM/QMâ€™ approach. Journal of Computational Chemistry, 2016, 37, 861-870.	3.3	26
24	Natural ionization orbitals for interpreting electron detachment processes. Journal of Chemical Physics, 2016, 144, 204117.	3.0	19
25	On the Driving Force of the Excited-State Proton Shuttle in the Green Fluorescent Protein: A Time-Dependent Density Functional Theory (TD-DFT) Study of the Intrinsic Reaction Path. Journal of Chemical Theory and Computation, 2016, 12, 4925-4933.	5.3	33
26	The Strongest Acid: Protonation of Carbon Dioxide. Angewandte Chemie - International Edition, 2016, 55, 1382-1386.	13.8	33
27	Second derivatives for approximate spin projection methods. Journal of Chemical Physics, 2015, 142, 054106.	3.0	16
28	Modeling the Photoelectron Spectra of MoNbO₂^{â€“} Accounting for Spin Contamination in Density Functional Theory. Journal of Physical Chemistry A, 2015, 119, 8744-8751.	2.5	18
29	Spin projection with double hybrid density functional theory. Journal of Chemical Physics, 2014, 141, 034108.	3.0	18
30	Computational Protocol for Modeling Thermochromic Molecular Crystals: Salicylidene Aniline As a Case Study. Journal of Chemical Theory and Computation, 2014, 10, 5577-5585.	5.3	44
31	Communication: An efficient analytic gradient theory for approximate spin projection methods. Journal of Chemical Physics, 2013, 138, 101101.	3.0	26
32	Improved Predictorâ€“Corrector Integrators For Evaluating Reaction Path Curvature. Journal of Chemical Theory and Computation, 2013, 9, 1481-1488.	5.3	27
33	Divalent pseudoatoms for modeling Si(100) surfaces. Journal of Chemical Physics, 2013, 139, 164708.	3.0	3
34	Using Efficient Predictor-Corrector Reaction Path Integrators for Studies Involving Projected Frequencies. Journal of Chemical Theory and Computation, 2012, 8, 5013-5019.	5.3	6
35	Thirty Years of Geometry Optimization in Quantum Chemistry and Beyond: A Tribute to Berny Schlegel. Journal of Chemical Theory and Computation, 2012, 8, 4853-4855.	5.3	2
36	Integrating steepest-descent reaction pathways for large molecules. Journal of Chemical Physics, 2011, 134, 204103.	3.0	31

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37	QM:QM embedding using electronic densities within an ONIOM framework: Energies and analytic gradients. Journal of Chemical Physics, 2011, 135, 014105.	3.0	20
38	Insights into Working Principles of Ruthenium Polypyridyl Dye-Sensitized Solar Cells from First Principles Modeling. Journal of Physical Chemistry C, 2011, 115, 4297-4306.	3.1	71
39	Steepest descent reaction path integration using a first-order predictorâ€“corrector method. Journal of Chemical Physics, 2010, 133, 224101.	3.0	63
40	ONIOM-based QM:QM electronic embedding method using LÃ¶wdin atomic charges: Energies and analytic gradients. Journal of Chemical Physics, 2010, 132, 114107.	3.0	37
41	First Principles Modeling of Eosin-Loaded ZnO Films: A Step toward the Understanding of Dye-Sensitized Solar Cell Performances. Journal of the American Chemical Society, 2009, 131, 14290-14298.	13.7	124
42	Applications and assessment of QM:QM electronic embedding using generalized asymmetric Mulliken atomic charges. Journal of Chemical Physics, 2008, 129, 145101.	3.0	25
43	QM:QM electronic embedding using Mulliken atomic charges: Energies and analytic gradients in an ONIOM framework. Journal of Chemical Physics, 2008, 128, 034107.	3.0	81
44	Archetypical Modeling and Amphiphilic Behavior of Cobalt(II)-Containing Soft-Materials with Asymmetric Tridentate Ligands. Inorganic Chemistry, 2007, 46, 9808-9818.	4.0	44
45	Amphiphilic and Magnetic Properties of a New Class of Clusterâ€Bearing [L₂Cu₄(Î¼₄â€O)(Î¼₂â€carboxylato)₄] Soft Materials. Chemistry - A European Journal, 2007, 13, 9948-9956.	3.3	25
46	Structural, spectroscopic, and electrochemical behavior of trans-phenolato cobalt(iii) complexes of asymmetric NNâ€²O ligands as archetypes for metallomesogens. Dalton Transactions, 2006, , 2517-2525.	3.3	55
47	Chemical failure modes of AlQ3-based OLEDs: AlQ3 hydrolysis. Physical Chemistry Chemical Physics, 2006, 8, 1371.	2.8	63
48	Structural and Electronic Behavior of Unprecedented Five-Coordinate Iron(III) and Gallium(III) Complexes with a New Phenol-Rich Electroactive Ligand. Inorganic Chemistry, 2006, 45, 955-957.	4.0	55
49	Hydrogen-Bonding Interactions in Peptide Nucleic Acid and Deoxyribonucleic Acid:â€‰ A Comparative Study. Journal of Physical Chemistry B, 2006, 110, 3336-3343.	2.6	20
50	First principles determination of 99Ru chemical shifts using moderately sized basis sets. Computational and Theoretical Chemistry, 2005, 724, 45-52.	1.5	6
51	Theoretical Investigation of Uranyl Dihydroxide: Oxo Ligand Exchange, Water Catalysis, and Vibrational Spectra. ChemInform, 2005, 36, no.	0.0	0
52	Theoretical Investigation of Uranyl Dihydroxide:Â Oxo Ligand Exchange, Water Catalysis, and Vibrational Spectra. Journal of Physical Chemistry A, 2005, 109, 8579-8586.	2.5	35
53	Influence of Ligand Rigidity and Ring Substitution on the Structural and Electronic Behavior of Trivalent Iron and Gallium Complexes with Asymmetric Tridentate Ligands. Inorganic Chemistry, 2005, 44, 7414-7422.	4.0	80
54	Using Hessian Updating To Increase the Efficiency of a Hessian Based Predictor-Corrector Reaction Path Following Method. Journal of Chemical Theory and Computation, 2005, 1, 61-69.	5.3	810

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55	Finding minima, transition states, and following reaction pathways on ab initio potential energy surfaces. , 2005, , 195-249.		266
56	Combined Experimental and Computational Investigation of the Mechanism of Nickel-Catalyzed Three-Component Addition Processes. Organometallics, 2004, 23, 4636-4646.	2.3	106
57	Accurate reaction paths using a Hessian based predictorâ€“corrector integrator. Journal of Chemical Physics, 2004, 120, 9918-9924.	3.0	796
58	Following Reaction Pathways Using a Damped Classical Trajectory Algorithm. Journal of Physical Chemistry A, 2002, 106, 165-169.	2.5	63
59	Theoretical investigation of substituent effects on the siliconâ€“metal bond for a series of transition metal-substituted base-stabilized silylene complexes. Polyhedron, 2001, 20, 209-213.	2.2	7