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	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
2	Accurate reaction paths using a Hessian based predictorâ€“corrector integrator. Journal of Chemical Physics, 2004, 120, 9918-9924.	3.0	796
3	Finding minima, transition states, and following reaction pathways on ab initio potential energy surfaces. , 2005, , 195-249.		266
4	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
5	Combined Experimental and Computational Investigation of the Mechanism of Nickel-Catalyzed Three-Component Addition Processes. Organometallics, 2004, 23, 4636-4646.	2.3	106
6	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
7	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
8	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
9	Following Reaction Pathways Using a Damped Classical Trajectory Algorithm. Journal of Physical Chemistry A, 2002, 106, 165-169.	2.5	63
10	Chemical failure modes of AlQ3-based OLEDs: AlQ3 hydrolysis. Physical Chemistry Chemical Physics, 2006, 8, 1371.	2.8	63
11	Steepest descent reaction path integration using a first-order predictorâ€“corrector method. Journal of Chemical Physics, 2010, 133, 224101.	3.0	63
12	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
13	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
14	Archetypical Modeling and Amphiphilic Behavior of Cobalt(II)-Containing Soft-Materials with Asymmetric Tridentate Ligands. Inorganic Chemistry, 2007, 46, 9808-9818.	4.0	44
15	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
16	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
17	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
18	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

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19	The Strongest Acid: Protonation of Carbon Dioxide. Angewandte Chemie - International Edition, 2016, 55, 1382-1386.	13.8	33
20	Integrating steepest-descent reaction pathways for large molecules. Journal of Chemical Physics, 2011, 134, 204103.	3.0	31
21	Experimental and Theoretical Evidence for Nitrogenâ€“Fluorine Halogen Bonding in Silver-Initiated Radical Fluorinations. ACS Catalysis, 2019, 9, 3322-3326.	11.2	29
22	Improved Predictorâ€“Corrector Integrators For Evaluating Reaction Path Curvature. Journal of Chemical Theory and Computation, 2013, 9, 1481-1488.	5.3	27
23	Communication: An efficient analytic gradient theory for approximate spin projection methods. Journal of Chemical Physics, 2013, 138, 101101.	3.0	26
24	Modeling emission features of salicylidene aniline molecular crystals: A QM/QMâ€™ approach. Journal of Computational Chemistry, 2016, 37, 861-870.	3.3	26
25	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
26	Applications and assessment of QM:QM electronic embedding using generalized asymmetric Mulliken atomic charges. Journal of Chemical Physics, 2008, 129, 145101.	3.0	25
27	Electronic and Molecular Structures of the CeB₆ Monomer. Journal of Physical Chemistry A, 2019, 123, 2040-2048.	2.5	22
28	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
29	QM:QM embedding using electronic densities within an ONIOM framework: Energies and analytic gradients. Journal of Chemical Physics, 2011, 135, 014105.	3.0	20
30	High-resolution photoelectron spectroscopy of TiO3H2â^': Probing the TiO2â^' + H2O dissociative adduct. Journal of Chemical Physics, 2018, 148, 222810.	3.0	20
31	Exceptionally Complex Electronic Structures of Lanthanide Oxides and Small Molecules. Accounts of Chemical Research, 2019, 52, 3265-3273.	15.6	20
32	Natural ionization orbitals for interpreting electron detachment processes. Journal of Chemical Physics, 2016, 144, 204117.	3.0	19
33	Spin projection with double hybrid density functional theory. Journal of Chemical Physics, 2014, 141, 034108.	3.0	18
34	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
35	Second derivatives for approximate spin projection methods. Journal of Chemical Physics, 2015, 142, 054106.	3.0	16
36	Explaining the MoVO4â^' photoelectron spectrum: Rationalization of geometric and electronic structure. Journal of Chemical Physics, 2017, 146, 104301.	3.0	14

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37	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
38	On approximate projection models. Molecular Physics, 2019, 117, 1421-1429.	1.7	13
39	Dispersion-Controlled Regioselective Acid-Catalyzed Intramolecular Hydroindolation of cis-Methindolylstyrenes To Access Tetrahydrobenzo[cd]indoles. Organic Letters, 2019, 21, 1574-1577.	4.6	10
40	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
41	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
42	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
43	Versatile New Reagent for Nitrosation under Mild Conditions. Organic Letters, 2021, 23, 3253-3258.	4.6	8
44	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
45	Enhanced Reactivity for Aromatic Bromination via Halogen Bonding with Lactic Acid Derivatives. Journal of Organic Chemistry, 2022, 87, 8492-8502.	3.2	7
46	First principles determination of 99Ru chemical shifts using moderately sized basis sets. Computational and Theoretical Chemistry, 2005, 724, 45-52.	1.5	6
47	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
48	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
49	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
50	Î”SCF Dyson orbitals and pole strengths from natural ionization orbitals. Journal of Chemical Physics, 2021, 154, 084104.	3.0	5
51	Divalent pseudoatoms for modeling Si(100) surfaces. Journal of Chemical Physics, 2013, 139, 164708.	3.0	3
52	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
53	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
54	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

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55	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
56	Aiming toward an Effective Hispanic-Serving Chemistry Curriculum. ACS Symposium Series, 2019, , 49-66.	0.5	1
57	On the linear geometry of lanthanide hydroxide (Ln-OH, Ln = Laâ€“Lu). Physical Chemistry Chemical Physics, 2019, 21, 21890-21897.	2.8	1
58	Theoretical Investigation of Uranyl Dihydroxide: Oxo Ligand Exchange, Water Catalysis, and Vibrational Spectra. ChemInform, 2005, 36, no.	0.0	0
59	A density functional theory investigation of the reaction of water with Ce2Oâ‚‚. Computational and Theoretical Chemistry, 2022, 1209, 113603.	2.5	0