Magnus W D Hanson-Heine

List of Publications by Year
in descending order

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42 papers	3,950 citations	430874 18 h-index	265206 42 g-index
43 all docs	43 docs citations	43 times ranked	4763 citing authors

#	Article	IF	Citations
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
2	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
3	Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction. Chemical Reviews, 2020, 120, 7152-7218.	47.7	205
4	Assessment of time-dependent density functional theory with the restricted excitation space approximation for excited state calculations of large systems. Molecular Physics, 2018, 116, 1452-1459.	1.7	64
5	Calculating excited state properties using Kohn-Sham density functional theory. Journal of Chemical Physics, 2013, 138, 064101.	3.0	47
6	Photoaquation Mechanism of Hexacyanoferrate(II) Ions: Ultrafast 2D UV and Transient Visible and IR Spectroscopies. Journal of the American Chemical Society, 2017, 139, 7335-7347.	13.7	43
7	Investigating the Calculation of Anharmonic Vibrational Frequencies Using Force Fields Derived from Density Functional Theory. Journal of Physical Chemistry A, 2012, 116, 4417-4425.	2.5	42
8	Basis sets for the calculation of core-electron binding energies. Chemical Physics Letters, 2018, 699, 279-285.	2.6	32
9	Kohn-Sham density functional theory calculations of non-resonant and resonant x-ray emission spectroscopy. Journal of Chemical Physics, 2017, 146, .	3.0	29
10	Kernel Methods for Predicting Yields of Chemical Reactions. Journal of Chemical Information and Modeling, 2022, 62, 2077-2092.	5.4	27
11	Photochemical Dihydrogen Production Using an Analogue of the Active Site of [NiFe] Hydrogenase. Inorganic Chemistry, 2014, 53, 4430-4439.	4.0	26
12	Examining the impact of harmonic correlation on vibrational frequencies calculated in localized coordinates. Journal of Chemical Physics, 2015, 143, 164104.	3.0	26
13	Monitoring the Formation and Reactivity of Organometallic Alkane and Fluoroalkane Complexes with Silanes and Xe Using Time-Resolved X-ray Absorption Fine Structure Spectroscopy. Journal of the American Chemical Society, 2019, 141, 11471-11480.	13.7	25
14	Can aliphatic anchoring groups be utilised with dyes for p-type dye sensitized solar cells?. Dalton Transactions, 2016, 45, 7708-7719.	3.3	24
15	Intermediate vibrational coordinate localization with harmonic coupling constraints. Journal of Chemical Physics, 2016, 144, 204116.	3.0	23
16	Dimers of acetic acid in helium nanodroplets. Physical Chemistry Chemical Physics, 2019, 21, 13950-13958.	2.8	23
17	Rapid anharmonic vibrational corrections derived from partial Hessian analysis. Journal of Chemical Physics, 2012, 136, 224102.	3.0	20
18	Simulation of Two-Dimensional Infrared Spectroscopy of Peptides Using Localized Normal Modes. Journal of Chemical Theory and Computation, 2016, 12, 1905-1918.	5.3	20

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19	Infrared Spectroscopy of NaCl(CH₃OH)_n Complexes in Helium Nanodroplets. Journal of Physical Chemistry A, 2016, 120, 8085-8092.	2.5	17
20	Benchmarking DFT-D Dispersion Corrections for Anharmonic Vibrational Frequencies and Harmonic Scaling Factors. Journal of Physical Chemistry A, 2019, 123, 9800-9808.	2.5	16
21	Calculating singlet excited states: Comparison with fast time-resolved infrared spectroscopy of coumarins. Journal of Chemical Physics, 2015, 142, 154119.	3.0	14
22	Static correlation in vibrational frequencies studied using thermally-assisted-occupation density functional theory. Chemical Physics Letters, 2020, 739, 137012.	2.6	13
23	Dewar Benzenoids Discovered In Carbon Nanobelts. Journal of Physical Chemistry Letters, 2020, 11, 3769-3772.	4.6	13
24	Reduced Basis Set Dependence in Anharmonic Frequency Calculations Involving Localized Coordinates. Journal of Chemical Theory and Computation, 2018, 14, 1277-1285.	5.3	12
25	Computational chemistry experiments performed directly on a blockchain virtual computer. Chemical Science, 2020, 11, 4644-4647.	7.4	11
26	Density functional theory calculations of the non-resonant and resonant X-ray emission spectroscopy of carbon fullerenes and nanotubes. Chemical Physics Letters, 2018, 696, 119-124.	2.6	10
27	A scaled CIS(D) based method for the calculation of valence and core electron ionization energies. Journal of Chemical Physics, 2019, 151, 034104.	3.0	10
28	MÃ¶bius and HÃ¼ckel Cyclacenes with Dewar and Ladenburg Defects. Journal of Physical Chemistry A, 2020, 124, 5408-5414.	2.5	10
29	Câ€“F Bond Activation of a Perfluorinated Ligand Leading to Nucleophilic Fluorination of an Organic Electrophile. Organometallics, 2020, 39, 2116-2124.	2.3	10
30	A combined time-resolved infrared and density functional theory study of the lowest excited states of 9-fluorenone and 2-naphthaldehyde. Chemical Physics, 2018, 512, 44-52.	1.9	9
31	Spectroscopic and structural analysis of mixed carbon dioxide and fluorinated methane clusters. Chemical Physics Letters, 2015, 638, 191-195.	2.6	8
32	Competing Pathways in the Photochemistry of Ru(H)₂(CO)(PPh₃)₃. Organometallics, 2018, 37, 855-868.	2.3	8
33	The effect of coordination of alkanes, Xe and CO₂ (Î·¹-OCO) on changes in spin state and reactivity in organometallic chemistry: a combined experimental and theoretical study of the photochemistry of CpMn(CO)₃. Faraday Discussions, 2019, 220, 86-104.	3.2	7
34	The impact of sulfur functionalisation on nitrogen-based ionic liquid cations. Chemical Communications, 2018, 54, 11403-11406.	4.1	6
35	Uncontracted core Pople basis sets in vibrational frequency calculations. International Journal of Quantum Chemistry, 2018, 118, e25761.	2.0	4
36	Electronically excited state geometries and vibrational frequencies calculated using the algebraic diagrammatic construction scheme for the polarization propagator. Chemical Physics Letters, 2019, 726, 62-68.	2.6	3

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37	Excited-State Vibrational Frequencies: Restricted Virtual Space Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2019, 123, 2949-2956.	2.5	3
38	Calculating with Permanent Marker: How Blockchains Record Immutable Mistakes in Computational Chemistry. Journal of Physical Chemistry Letters, 2020, 11, 6618-6620.	4.6	3
39	Integrated Multistep Photochemical and Thermal Continuous Flow Reactions: Production of Bicyclic Lactones with Kilogram Productivity. Organic Process Research and Development, 2021, 25, 2052-2059.	2.7	3
40	Influence of molecular design on radical spin multiplicity: characterisation of BODIPY dyad and triad radical anions. Physical Chemistry Chemical Physics, 2020, 22, 4429-4438.	2.8	2
41	Wavelength dependent photoextrusion and tandem photo-extrusion reactions of ninhydrin bis-acetals for the synthesis of 8-ring lactones, benzocyclobutenes and orthoanhydrides. Chemical Communications, 2022, 58, 1546-1549.	4.1	2
42	Reduced Two-Electron Interactions in Anharmonic Molecular Vibrational Calculations Involving Localized Normal Coordinates. Journal of Chemical Theory and Computation, 2021, 17, 4383-4391.	5.3	1