Magnus W D Hanson-Heine

List of Publications by Year
in descending order

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42 papers	3,950 citations	430442 18 h-index	264894 42 g-index
43 all docs	43 docs citations	43 times ranked	4763 citing authors

#	Article	IF	Citations
1	Kernel Methods for Predicting Yields of Chemical Reactions. Journal of Chemical Information and Modeling, 2022, 62, 2077-2092.	2.5	27
2	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.	2.2	2
3	Reduced Two-Electron Interactions in Anharmonic Molecular Vibrational Calculations Involving Localized Normal Coordinates. Journal of Chemical Theory and Computation, 2021, 17, 4383-4391.	2.3	1
4	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
5	Integrated Multistep Photochemical and Thermal Continuous Flow Reactions: Production of Bicyclic Lactones with Kilogram Productivity. Organic Process Research and Development, 2021, 25, 2052-2059.	1.3	3
6	Static correlation in vibrational frequencies studied using thermally-assisted-occupation density functional theory. Chemical Physics Letters, 2020, 739, 137012.	1.2	13
7	Calculating with Permanent Marker: How Blockchains Record Immutable Mistakes in Computational Chemistry. Journal of Physical Chemistry Letters, 2020, 11, 6618-6620.	2.1	3
8	MÃ¶bius and HÃ¼ckel Cyclacenes with Dewar and Ladenburg Defects. Journal of Physical Chemistry A, 2020, 124, 5408-5414.	1.1	10
9	Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction. Chemical Reviews, 2020, 120, 7152-7218.	23.0	205
10	Influence of molecular design on radical spin multiplicity: characterisation of BODIPY dyad and triad radical anions. Physical Chemistry Chemical Physics, 2020, 22, 4429-4438.	1.3	2
11	Dewar Benzenoids Discovered In Carbon Nanobelts. Journal of Physical Chemistry Letters, 2020, 11, 3769-3772.	2.1	13
12	Câ€“F Bond Activation of a Perfluorinated Ligand Leading to Nucleophilic Fluorination of an Organic Electrophile. Organometallics, 2020, 39, 2116-2124.	1.1	10
13	Computational chemistry experiments performed directly on a blockchain virtual computer. Chemical Science, 2020, 11, 4644-4647.	3.7	11
14	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.	6.6	25
15	A scaled CIS(D) based method for the calculation of valence and core electron ionization energies. Journal of Chemical Physics, 2019, 151, 034104.	1.2	10
16	Benchmarking DFT-D Dispersion Corrections for Anharmonic Vibrational Frequencies and Harmonic Scaling Factors. Journal of Physical Chemistry A, 2019, 123, 9800-9808.	1.1	16
17	Dimers of acetic acid in helium nanodroplets. Physical Chemistry Chemical Physics, 2019, 21, 13950-13958.	1.3	23
18	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.	1.2	3

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19	Excited-State Vibrational Frequencies: Restricted Virtual Space Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2019, 123, 2949-2956.	1.1	3
20	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.	1.6	7
21	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.	1.2	10
22	Reduced Basis Set Dependence in Anharmonic Frequency Calculations Involving Localized Coordinates. Journal of Chemical Theory and Computation, 2018, 14, 1277-1285.	2.3	12
23	Competing Pathways in the Photochemistry of Ru(H)₂(CO)(PPh₃)₃. Organometallics, 2018, 37, 855-868.	1.1	8
24	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.	0.8	64
25	Basis sets for the calculation of core-electron binding energies. Chemical Physics Letters, 2018, 699, 279-285.	1.2	32
26	Uncontracted core Pople basis sets in vibrational frequency calculations. International Journal of Quantum Chemistry, 2018, 118, e25761.	1.0	4
27	The impact of sulfur functionalisation on nitrogen-based ionic liquid cations. Chemical Communications, 2018, 54, 11403-11406.	2.2	6
28	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.	0.9	9
29	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.	6.6	43
30	Kohn-Sham density functional theory calculations of non-resonant and resonant x-ray emission spectroscopy. Journal of Chemical Physics, 2017, 146, .	1.2	29
31	Intermediate vibrational coordinate localization with harmonic coupling constraints. Journal of Chemical Physics, 2016, 144, 204116.	1.2	23
32	Can aliphatic anchoring groups be utilised with dyes for p-type dye sensitized solar cells?. Dalton Transactions, 2016, 45, 7708-7719.	1.6	24
33	Infrared Spectroscopy of NaCl(CH₃OH)_n Complexes in Helium Nanodroplets. Journal of Physical Chemistry A, 2016, 120, 8085-8092.	1.1	17
34	Simulation of Two-Dimensional Infrared Spectroscopy of Peptides Using Localized Normal Modes. Journal of Chemical Theory and Computation, 2016, 12, 1905-1918.	2.3	20
35	Examining the impact of harmonic correlation on vibrational frequencies calculated in localized coordinates. Journal of Chemical Physics, 2015, 143, 164104.	1.2	26
36	Calculating singlet excited states: Comparison with fast time-resolved infrared spectroscopy of coumarins. Journal of Chemical Physics, 2015, 142, 154119.	1.2	14

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37	Spectroscopic and structural analysis of mixed carbon dioxide and fluorinated methane clusters. Chemical Physics Letters, 2015, 638, 191-195.	1.2	8
38	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
39	Photochemical Dihydrogen Production Using an Analogue of the Active Site of [NiFe] Hydrogenase. Inorganic Chemistry, 2014, 53, 4430-4439.	1.9	26
40	Calculating excited state properties using Kohn-Sham density functional theory. Journal of Chemical Physics, 2013, 138, 064101.	1.2	47
41	Rapid anharmonic vibrational corrections derived from partial Hessian analysis. Journal of Chemical Physics, 2012, 136, 224102.	1.2	20
42	Investigating the Calculation of Anharmonic Vibrational Frequencies Using Force Fields Derived from Density Functional Theory. Journal of Physical Chemistry A, 2012, 116, 4417-4425.	1.1	42