Krishnan Raghavachari

List of Publications by Year
in descending order

154 papers	23,177 citations	61977 43 h-index	7517 151 g-index
158 all docs	158 docs citations	158 times ranked	11194 citing authors

#	Article	IF	Citations
1	A fifth-order perturbation comparison of electron correlation theories. Chemical Physics Letters, 1989, 157, 479-483.	2.6	7,448
2	Gaussian-3 (G3) theory for molecules containing first and second-row atoms. Journal of Chemical Physics, 1998, 109, 7764-7776.	3.0	2,746
3	Assessment of Gaussian-2 and density functional theories for the computation of enthalpies of formation. Journal of Chemical Physics, 1997, 106, 1063-1079.	3.0	2,015
4	Gaussian-4 theory. Journal of Chemical Physics, 2007, 126, 084108.	3.0	1,741
5	Gaussian-3 theory using reduced Mo/ller-Plesset order. Journal of Chemical Physics, 1999, 110, 4703-4709.	3.0	1,201
6	Assessment of Gaussian-3 and density functional theories for a larger experimental test set. Journal of Chemical Physics, 2000, 112, 7374-7383.	3.0	711
7	Gaussian-4 theory using reduced order perturbation theory. Journal of Chemical Physics, 2007, 127, 124105.	3.0	598
8	Assessment of Gaussian-2 and density functional theories for the computation of ionization potentials and electron affinities. Journal of Chemical Physics, 1998, 109, 42-55.	3.0	536
9	Size-consistent Brueckner theory limited to double substitutions. Chemical Physics Letters, 1989, 164, 185-192.	2.6	478
10	Gaussian-3X (G3X) theory: Use of improved geometries, zero-point energies, and Hartreeâ€“Fock basis sets. Journal of Chemical Physics, 2001, 114, 108.	3.0	477
11	Assessment of Gaussian-3 and density-functional theories on the G3/05 test set of experimental energies. Journal of Chemical Physics, 2005, 123, 124107.	3.0	320
12	Accurate Composite and Fragment-Based Quantum Chemical Models for Large Molecules. Chemical Reviews, 2015, 115, 5643-5677.	47.7	225
13	Gn theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 810-825.	14.6	189
14	Molecules-in-Molecules: An Extrapolated Fragment-Based Approach for Accurate Calculations on Large Molecules and Materials. Journal of Chemical Theory and Computation, 2011, 7, 1336-1343.	5.3	177
15	Gaussianâ€2 theory: Use of higher level correlation methods, quadratic configuration interaction geometries, and secondâ€order Mo/llerâ€“Plesset zeroâ€point energies. Journal of Chemical Physics, 1995, 103, 4192-4200.	3.0	146
16	Anion Binding in Solution: Beyond the Electrostatic Regime. CheM, 2017, 3, 411-427.	11.7	129
17	Gaussian-3 and related methods for accurate thermochemistry. Theoretical Chemistry Accounts, 2002, 108, 61-70.	1.4	122
18	Gaussian-3 theory using scaled energies. Journal of Chemical Physics, 2000, 112, 1125-1132.	3.0	119

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19	Anions Stabilize Each Other inside Macrocyclic Hosts. Angewandte Chemie - International Edition, 2016, 55, 14057-14062.	13.8	115
20	Silicon Epoxide: Unexpected Intermediate during Silicon Oxide Formation. Physical Review Letters, 1998, 81, 3908-3911.	7.8	112
21	Many-Overlapping-Body (MOB) Expansion: A Generalized Many Body Expansion for Nondisjoint Monomers in Molecular Fragmentation Calculations of Covalent Molecules. Journal of Chemical Theory and Computation, 2012, 8, 2669-2675.	5.3	104
22	Aromatic and Aliphatic CH Hydrogen Bonds Fight for Chloride while Competing Alongside Ion Pairing within Triazolophanes. Chemistry - A European Journal, 2011, 17, 312-321.	3.3	98
23	Role of Interdimer Interactions inNH3Dissociation onSi(100)â^'(2Ã—1). Physical Review Letters, 2001, 86, 1046-1049.	7.8	96
24	Well-Defined Nanographeneâ€“Rhenium Complex as an Efficient Electrocatalyst and Photocatalyst for Selective CO₂ Reduction. Journal of the American Chemical Society, 2017, 139, 3934-3937.	13.7	95
25	Allosteric Control of Photofoldamers for Selecting between Anion Regulation and Double-to-Single Helix Switching. Journal of the American Chemical Society, 2018, 140, 17711-17723.	13.7	90
26	Inâ€vitro and Inâ€vivo Photocatalytic Cancer Therapy with Biocompatible Iridium(III) Photocatalysts. Angewandte Chemie - International Edition, 2021, 60, 9474-9479.	13.8	89
27	A Model for the pH-Dependent Selectivity of the Oxygen Reduction Reaction Electrocatalyzed by N-Doped Graphitic Carbon. Journal of the American Chemical Society, 2016, 138, 13923-13929.	13.7	88
28	Theoretical Thermochemistry for Organic Molecules: Development of the Generalized Connectivity-Based Hierarchy. Journal of Chemical Theory and Computation, 2011, 7, 2094-2103.	5.3	77
29	Structures of Mo2Oyâ^' and Mo2Oy (y=2, 3, and 4) studied by anion photoelectron spectroscopy and density functional theory calculations. Journal of Chemical Physics, 2005, 122, 094313.	3.0	75
30	Chlorination of hydrogen-terminated silicon (111) surfaces. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2005, 23, 1100-1106.	2.1	71
31	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
32	Electrostatic and Allosteric Cooperativity in Ion-Pair Binding: A Quantitative and Coupled Experimentâ€“Theory Study with Arylâ€“Triazoleâ€“Ether Macrocycles. Journal of the American Chemical Society, 2015, 137, 9746-9757.	13.7	69
33	Electrocatalytic Oxygen Activation by Carbanion Intermediates of Nitrogen-Doped Graphitic Carbon. Journal of the American Chemical Society, 2014, 136, 3358-3361.	13.7	68
34	Investigation of Gaussian4 Theory for Transition Metal Thermochemistry. Journal of Physical Chemistry A, 2009, 113, 5170-5175.	2.5	65
35	The structure of nâ€alkanes: High precision ab initio calculation and relation to vibrational spectra. Journal of Chemical Physics, 1986, 84, 6872-6878.	3.0	64
36	Extrapolation to the Gold-Standard in Quantum Chemistry: Computationally Efficient and Accurate CCSD(T) Energies for LargeÂMolecules Using an Automated Thermochemical Hierarchy. Journal of Chemical Theory and Computation, 2013, 9, 3986-3994.	5.3	64

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37	Atomic Layer Deposition Growth Reactions of Al2O3 on Si(100)-2Ã—1. Journal of Physical Chemistry B, 2004, 108, 4058-4062.	2.6	60
38	Two levels of conformational pre-organization consolidate strong CH hydrogen bonds in chlorideâ€“triazolophane complexes. Chemical Communications, 2011, 47, 5979.	4.1	60
39	Flexibility Coexists with Shape-Persistence in Cyanostar Macrocycles. Journal of the American Chemical Society, 2016, 138, 4843-4851.	13.7	53
40	Atomic layer deposition of Al2O3 on H-passivated Si. I. Initial surface reaction pathways with H/Si(100)-2Ã—1. Journal of Chemical Physics, 2003, 118, 10221-10226.	3.0	51
41	Strong CHâ‹…â‹…â‹…Halide Hydrogen Bonds from 1,2,3â€Triazoles Quantified Using Preâ€Organized and Shapeâ€Persistent Triazolophanes. ChemPhysChem, 2009, 10, 2535-2540.	2.1	50
42	An Overlooked yet Ubiquitous Fluoride Congenitor: Binding Bifluoride in Triazolophanes Using Computer-Aided Design. Journal of the American Chemical Society, 2014, 136, 5078-5089.	13.7	47
43	Quantum chemical studies of semiconductor surface chemistry using cluster models. Molecular Physics, 2004, 102, 381-393.	1.7	43
44	Unusual products observed in gas-phase WxOyâ¯+H2O and D2O reactions. Journal of Chemical Physics, 2009, 130, 124314.	3.0	42
45	Atomic layer deposition ofAl2O3on H-passivated Si:â€ƒAl(CH3)2OHsurface reactions withH/Si(100)â¯2Ã—1. Physical Review B, 2003, 68, .	3.2	41
46	From Atomic to Molecular Anions: A Neutral Receptor Captures Cyanide Using Strong Cï£¿H Hydrogen Bonds. Chemistry - A European Journal, 2011, 17, 9123-9129.	3.3	41
47	Connectivity-Based Hierarchy for Theoretical Thermochemistry: Assessment Using Wave Function-Based Methods. Journal of Physical Chemistry A, 2012, 116, 7531-7537.	2.5	41
48	New Insights on Photocatalytic H₂ Liberation from Water Using Transition-Metal Oxides: Lessons from Cluster Models of Molybdenum and Tungsten Oxides. Journal of the American Chemical Society, 2013, 135, 17039-17051.	13.7	41
49	Vibrational Circular Dichroism Spectra for Large Molecules through Molecules-in-Molecules Fragment-Based Approach. Journal of Chemical Theory and Computation, 2015, 11, 4238-4247.	5.3	40
50	Fragment-Based Approach for the Evaluation of NMR Chemical Shifts for Large Biomolecules Incorporating the Effects of the Solvent Environment. Journal of Chemical Theory and Computation, 2017, 13, 1147-1158.	5.3	40
51	Water reactivity with tungsten oxides: H2 production and kinetic traps. Journal of Chemical Physics, 2009, 131, 144302.	3.0	39
52	Electronic structures of MoWOyâ¯ and MoWOy determined by anion photoelectron spectroscopy and DFT calculations. Journal of Chemical Physics, 2009, 130, 124313.	3.0	39
53	Evaluation of Energy Gradients and Infrared Vibrational Spectra through Molecules-in-Molecules Fragment-Based Approach. Journal of Chemical Theory and Computation, 2015, 11, 950-961.	5.3	39
54	Addition of water to Al5O4â¯ determined by anion photoelectron spectroscopy and quantum chemical calculations. Journal of Chemical Physics, 2005, 122, 014313.	3.0	37

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55	Energy Decomposition Analysis of Proteinâ€“Ligand Interactions Using Molecules-in-Molecules Fragmentation-Based Method. Journal of Chemical Information and Modeling, 2019, 59, 3474-3484.	5.4	35
56	The Successful Merger of Theoretical Thermochemistry with Fragment-Based Methods in Quantum Chemistry. Accounts of Chemical Research, 2014, 47, 3596-3604.	15.6	34
57	Analysis of Different Fragmentation Strategies on a Variety of Large Peptides: Implementation of a Low Level of Theory in Fragment-Based Methods Can Be a Crucial Factor. Journal of Chemical Theory and Computation, 2015, 11, 2012-2023.	5.3	34
58	G4(MP2)-XK: A Variant of the G4(MP2)-6X Composite Method with Expanded Applicability for Main-Group Elements up to Radon. Journal of Chemical Theory and Computation, 2019, 15, 4478-4484.	5.3	34
59	Dimers of Dimers (DOD): A New Fragment-Based Method Applied to Large Water Clusters. Journal of Chemical Theory and Computation, 2014, 10, 58-67.	5.3	33
60	Theoretical Study of Proteinâ€“Ligand Interactions Using the Molecules-in-Molecules Fragmentation-Based Method. Journal of Chemical Theory and Computation, 2018, 14, 5143-5155.	5.3	33
61	Raman Optical Activity Spectra for Large Molecules through Molecules-in-Molecules Fragment-Based Approach. Journal of Chemical Theory and Computation, 2016, 12, 585-594.	5.3	32
62	Accurate pK_a Evaluations for Complex Bio-Organic Molecules in Aqueous Media. Journal of Chemical Theory and Computation, 2019, 15, 6025-6035.	5.3	31
63	Prediction of Accurate Thermochemistry of Medium and Large Sized Radicals Using Connectivity-Based Hierarchy (CBH). Journal of Chemical Theory and Computation, 2014, 10, 4342-4350.	5.3	30
64	Zero-Overlap Fluorophores for Fluorescent Studies at Any Concentration. Journal of the American Chemical Society, 2020, 142, 12167-12180.	13.7	30
65	Hydrogen adsorption on phosphorus-rich(2Ã—1)indium phosphide (001). Physical Review B, 2002, 65, .	3.2	29
66	Importance of Steric Effects in Cluster Models of Silicon Surface Chemistry:Â ONIOM Studies of the Atomic Layer Deposition (ALD) of Al2O3on H/Si(111)â€. Journal of Physical Chemistry A, 2004, 108, 2982-2987.	2.5	29
67	Termination of the W2Oyâ^'+H2O/D2Oâ†'W2Oy+1â^'+H2/D2 sequential oxidation reaction: An exploration of kinetic versus thermodynamic effects. Journal of Chemical Physics, 2009, 131, 144306.	3.0	29
68	Assessment of Fragmentation Strategies for Large Proteins Using the Multilayer Molecules-in-Molecules Approach. Journal of Chemical Theory and Computation, 2018, 14, 1383-1394.	5.3	29
69	Theoretical study of substituent effects on CH stretching frequencies. Journal of Chemical Physics, 1984, 81, 2717-2722.	3.0	28
70	Molybdenum Oxides versus Molybdenum Sulfides: Geometric and Electronic Structures of Mo₃X_y^{â^'} (X = O, S and y = 6, 9) Clusters. Journal of Physical Chemistry A, 2011, 115, 2291-2296.	2.5	28
71	Comparative study of water reactivity with Mo2Oyâ^' and W2Oyâ^' clusters: A combined experimental and theoretical investigation. Journal of Chemical Physics, 2014, 141, 104310.	3.0	28
72	Application of the Generalized Connectivity-Based Hierarchy to Biomonomers: Enthalpies of Formation of Cysteine and Methionine. Journal of Physical Chemistry A, 2013, 117, 4973-4980.	2.5	27

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73	Solving the Density Functional Conundrum: Elimination of Systematic Errors To Derive Accurate Reaction Enthalpies of Complex Organic Reactions. Organic Letters, 2017, 19, 2576-2579.	4.6	27
74	Heats of Formation for CrO, CrO2, and CrO3: An Extreme Challenge for Black-Box Composite Procedures. Journal of Chemical Theory and Computation, 2012, 8, 3159-3166.	5.3	26
75	Anions Stabilize Each Other inside Macrocyclic Hosts. Angewandte Chemie, 2016, 128, 14263-14268.	2.0	25
76	Applications of isodesmicâ€type reactions for computational thermochemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1501.	14.6	25
77	Hostâ€“Host Interactions Control Selfâ€assembly and Switching of Triple and Double Decker Stacks of Tricarbazole Macrocycles Coâ€assembled with antiâ€Electrostatic Bisulfate Dimers. Chemistry - A European Journal, 2018, 24, 9841-9852.	3.3	24
78	Inâ€vitro and Inâ€vivo Photocatalytic Cancer Therapy with Biocompatible Iridium(III) Photocatalysts. Angewandte Chemie, 2021, 133, 9560-9565.	2.0	24
79	Hydrogen evolution from water through metal sulfide reactions. Journal of Chemical Physics, 2013, 139, 204301.	3.0	23
80	C vs N: Which End of the Cyanide Anion Is a Better Hydrogen Bond Acceptor?. Journal of Physical Chemistry A, 2014, 118, 7418-7423.	2.5	22
81	Molecules-in-molecules fragment-based method for the evaluation of Raman spectra of large molecules. Molecular Physics, 2015, 113, 3057-3066.	1.7	22
82	Revealing the Hidden Costs of Organization in Hostâ€“Guest Chemistry Using Chloride-Binding Foldamers and Their Solvent Dependence. Journal of the American Chemical Society, 2022, 144, 1274-1287.	13.7	22
83	Singleâ€Cell Quantification of a Highly Biocompatible Dinuclear Iridium(III) Complex for Photocatalytic Cancer Therapy. Angewandte Chemie - International Edition, 2022, 61, .	13.8	22
84	Photosensitized [2+2]â€Cycloadditions of Alkenylboronates and Alkenes. Angewandte Chemie - International Edition, 2022, 61, e202200725.	13.8	22
85	Anionâ€Binding Macrocycles Operate Beyond the Electrostatic Regime: Interaction Distances Matter. Chemistry - A European Journal, 2018, 24, 14409-14417.	3.3	20
86	Proton Hop Paving the Way for Hydroxyl Migration: Theoretical Elucidation of Fluxionality in Transition-Metal Oxide Clusters. Journal of Physical Chemistry Letters, 2010, 1, 3066-3071.	4.6	19
87	Restricted-Open-Shell G4(MP2)-Type Procedures. Journal of Physical Chemistry A, 2016, 120, 9299-9304.	2.5	19
88	Multi-state amine sensing by electron transfers in a BODIPY probe. Organic and Biomolecular Chemistry, 2020, 18, 431-440.	2.8	19
89	Accurate and cost-effective NMR chemical shift predictions for proteins using a molecules-in-molecules fragmentation-based method. Physical Chemistry Chemical Physics, 2020, 22, 27781-27799.	2.8	19
90	Charge Transfer Across ONIOM QM:QM Boundaries: The Impact of Model System Preparation. Journal of Chemical Theory and Computation, 2010, 6, 3131-3136.	5.3	18

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91	Effective Molecular Descriptors for Chemical Accuracy at DFT Cost: Fragmentation, Error-Cancellation, and Machine Learning. Journal of Chemical Theory and Computation, 2020, 16, 4938-4950.	5.3	18
92	Infrared Intensities of Î½(Siâ”H) on H/Si(100)-2Ã—1:Â Effect of O Incorporation and Agglomeration. Journal of Physical Chemistry B, 2004, 108, 19388-19391.	2.6	17
93	Two Methanes are Better than One:â€‰ A Density Functional Theory Study of the Reactions of Mo₂O_y⁻ (y = 2â˜5) with Methane. Journal of Physical Chemistry A, 2007, 111, 8211-8217.	2.5	17
94	Insight into ethylene interactions with molybdenum suboxide cluster anions from photoelectron spectra of chemifragments. Journal of Chemical Physics, 2018, 148, 054308.	3.0	17
95	A comparison of stable carbonyls formed in the gas-phase reaction between group 10 atomic anions and methanol or methoxy radicals: Anion photoelectron spectroscopy and density functional theory calculations on HNiCOâ˜, PdCOâ˜, and PtCOâ˜. Journal of Chemical Physics, 2003, 119, 10591-10599.	3.0	16
96	The microscopic origin of optical phonon evolution during water oxidation of Si(100). Journal of Chemical Physics, 2003, 119, 2307-2313.	3.0	16
97	Moleculesâ€inâ€molecules fragmentâ€based method for the calculation of chiroptical spectra of large molecules: Vibrational circular dichroism and Raman optical activity spectra of alanine polypeptides. Chirality, 2016, 28, 755-768.	2.6	15
98	The striking influence of oxophilicity differences in heterometallic Moâ€“Mn oxide cluster reactions with water. Journal of Chemical Physics, 2020, 152, 054301.	3.0	15
99	Al5O4: A Superatom with Potential for New Materials Design. Journal of Chemical Theory and Computation, 2008, 4, 2011-2019.	5.3	14
100	Multiple Solutions to the Single-Reference CCSD Equations for NiH. Journal of Chemical Theory and Computation, 2010, 6, 2714-2720.	5.3	14
101	Basal Plane Fluorination of Graphene by XeF₂ via a Radical Cation Mechanism. Journal of Physical Chemistry Letters, 2015, 6, 3645-3649.	4.6	14
102	Hydrogen evolution from water reactions with molybdenum sulfide cluster anions. International Journal of Mass Spectrometry, 2018, 434, 193-201.	1.5	14
103	Eliminating Systematic Errors in DFT via Connectivity-Based Hierarchy: Accurate Bond Dissociation Energies of Biodiesel Methyl Esters. Journal of Physical Chemistry A, 2019, 123, 3543-3550.	2.5	14
104	Accurate and Computationally Efficient Prediction of Thermochemical Properties of Biomolecules Using the Generalized Connectivity-Based Hierarchy. Journal of Physical Chemistry B, 2014, 118, 9631-9643.	2.6	13
105	Direct Reduction of Alkyl Monohalides at Silver in Dimethylformamide: Effects of Position and Identity of the Halogen. ChemElectroChem, 2015, 2, 726-736.	3.4	13
106	G4 accuracy at DFT cost: unlocking accurate redox potentials for organic molecules using systematic error cancellation. Physical Chemistry Chemical Physics, 2020, 22, 4439-4452.	2.8	13
107	Accurate Thermochemistry for Organic Cations via Error Cancellation using Connectivity-Based Hierarchy. Journal of Physical Chemistry A, 2018, 122, 1807-1812.	2.5	12
108	Fragment-Based Approaches for Supramolecular Interaction Energies: Applications to Foldamers and Their Complexes with Anions. Journal of Chemical Theory and Computation, 2018, 14, 6226-6239.	5.3	12

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109	Role of weakly bound complexes in temperature-dependence and relative rates of MxOyâ˜ + H2O (M = Mo, W) reactions. Journal of Chemical Physics, 2016, 144, 074307.	3.0	11
110	A Grotthuss-like proton shuttle in the anomalous C₂H₃⁺carbocation: energetic and vibrational properties for isotopologues. Physical Chemistry Chemical Physics, 2016, 18, 29395-29411.	2.8	11
111	Redox â€œInnocenceâ€•of Re(I) in Electrochemical CO2 Reduction Catalyzed by Nanographeneâ€“Re Complexes. Inorganic Chemistry, 2018, 57, 10548-10556.	4.0	11
112	Highly Efficient Ir(III)â€Coumarin Photoâ€Redox Catalyst for Synergetic Multiâ€Mode Cancer Photoâ€Therapy. Chemistry - A European Journal, 2022, 28, .	3.3	11
113	Reactions of Atomic Hydrogen with the Hydroxide- and Amine-Functionalized Si(100)-2Ã—1 Surfaces: Accurate Modeling of Hydrogen Abstraction Reactions Using Density Functional Theory. Journal of Physical Chemistry C, 2014, 118, 8379-8386.	3.1	10
114	Molybdenum Oxide Cluster Anion Reactions with C₂H₄ and H₂O: Cooperativity and Chemifragmentation. Journal of Physical Chemistry A, 2018, 122, 41-52.	2.5	10
115	Hydrogen evolution from water using Moâ€“oxide clusters in the gas phase: DFT modeling of a complete catalytic cycle using a Mo₂O₄^{â˜}/Mo₂O₅^{â˜} cluster couple. Physical Chemistry Chemical Physics, 2016, 18, 25687-25692.	2.8	9
116	Quantum Mechanical Investigation of Three-Dimensional Activity Cliffs Using the Molecules-in-Molecules Fragmentation-Based Method. Journal of Chemical Information and Modeling, 2020, 60, 2924-2938.	5.4	9
117	A Fragmentation-Based Graph Embedding Framework for QM/ML. Journal of Physical Chemistry A, 2021, 125, 6872-6880.	2.5	9
118	Interaction of Lewis Acids with Si(100)-2Ã—1 and Ge(100)-2Ã—1 Surfaces. Journal of Physical Chemistry C, 2009, 113, 10146-10150.	3.1	8
119	Extending Molecular Lines on the Si(100)-2 Ã— 1 Surface: A Theoretical Study of the Effect of Allylic Mercaptan Adsorbates on Radical Chain Reactions. Journal of Physical Chemistry Letters, 2010, 1, 679-685.	4.6	8
120	Electrostatic Potential-Based Method of Balancing Charge Transfer Across ONIOM QM:QM Boundaries. Journal of Chemical Theory and Computation, 2014, 10, 4351-4359.	5.3	8
121	H₂S Reactivity on Oxygen-Deficient Heterotrimetallic Cores: Cluster Fluxionality Simulates Dynamic Aspects of Surface Chemical Reactions. Journal of Physical Chemistry A, 2016, 120, 466-472.	2.5	8
122	Amphiphile self-assembly dynamics at the solution-solid interface reveal asymmetry in head/tail desorption. Chemical Communications, 2018, 54, 10076-10079.	4.1	8
123	Phosphine Adsorption on the In-Rich InP(001) Surface:â€‰ Evidence of Surface Dative Bonds at Room Temperature. Langmuir, 2007, 23, 10109-10115.	3.5	7
124	Line Growth on the H/Si(100)-2 Ã— 1 Surface: Density Functional Study of Allylic Mercaptan Reaction Mechanisms. Journal of Physical Chemistry C, 2009, 113, 18817-18822.	3.1	7
125	Electronic Energies Are Not Enough: An Ion Mobility-Aided, Quantum Chemical Benchmark Analysis of H⁺GPGG Conformers. Journal of Chemical Theory and Computation, 2018, 14, 5406-5418.	5.3	7
126	Mo Insertion into the H₂ Bond in Mo_xS_y^{â€“} + H₂ Reactions. Journal of Physical Chemistry A, 2019, 123, 7261-7269.	2.5	7

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127	Solution-Mediated Annealing Pathways Are Critical for Supramolecular Ordering of Complex Macrocycles at Surfaces. Journal of Physical Chemistry C, 2020, 124, 6689-6699.	3.1	7
128	Aromatic Fragmentation Based on a Ring Overlap Scheme: An Algorithm for Large Polycyclic Aromatic Hydrocarbons Using the Molecules-in-Molecules Fragmentation-Based Method. Journal of Chemical Theory and Computation, 2020, 16, 2160-2171.	5.3	7
129	Photosensitized [2+2]â€Cycloadditions of Alkenylboronates and Alkenes. Angewandte Chemie, 2022, 134, .	2.0	7
130	Breaking a bottleneck: Accurate extrapolation to â€œgold standardâ€•CCSD(T) energies for large open shell organic radicals at reduced computational cost. Journal of Computational Chemistry, 2016, 37, 286-295.	3.3	6
131	Bond Activation and Hydrogen Evolution from Water through Reactions with M3S4 (M = Mo, W) and W3S3 Anionic Clusters. Journal of Physical Chemistry A, 2017, 121, 1760-1767.	2.5	6
132	Understanding the Origin of 2D Self-Assembly of Tricarbazole Macrocycles: An Integrated Quantum Mechanical/Molecular Dynamics Study. Journal of Physical Chemistry C, 2019, 123, 17616-17623.	3.1	6
133	Coupling Constants, High Spin, and Broken Symmetry States of Organic Radicals: an Assessment of the Molecules-in-Molecules Fragmentation-Based Method. Journal of Chemical Theory and Computation, 2019, 15, 5998-6009.	5.3	6
134	In-Rich Surface Growth on P-Rich InP(001) (2 Ã— 1) Surface:â€‰ Structural and Mechanistic Study. Journal of Physical Chemistry C, 2008, 112, 6022-6026.	3.1	5
135	Electronic structures and water reactivity of mixed metal sulfide cluster anions. Journal of Chemical Physics, 2014, 141, 074305.	3.0	5
136	Comparative assessment of QM-based and MM-based models for prediction of proteinâ€“ligand binding affinity trends. Physical Chemistry Chemical Physics, 2022, 24, 14525-14537.	2.8	5
137	Predicting PH vibrations of gas phase molecules and surfaceâ€adsorbed species using bond lengthâ€frequency correlations. Journal of Computational Chemistry, 2009, 30, 1872-1881.	3.3	4
138	Charge redistribution in QM:QM ONIOM model systems: a constrained density functional theory approach. Molecular Physics, 2017, 115, 2813-2822.	1.7	4
139	Mechanistic Role of Two-State Reactivity in a Molecular MoS₂ Edge-Site Analogue for Hydrogen Evolution Electrocatalysis. Inorganic Chemistry, 2018, 57, 9167-9174.	4.0	4
140	Electrostatically embedded moleculesâ€inâ€molecules approach and its application to molecular clusters. Journal of Computational Chemistry, 2021, 42, 719-734.	3.3	4
141	Three-Dimensional Convolutional Neural Networks Utilizing Molecular Topological Features for Accurate Atomization Energy Predictions. Journal of Chemical Theory and Computation, 2022, 18, 2132-2143.	5.3	4
142	Temperature-Programmed Desorption (TPD) and Density Functional Theory (DFT) Study Comparing the Adsorption of Ethyl Halides on the Si(100) Surface. Journal of Physical Chemistry C, 2017, 121, 7208-7213.	3.1	3
143	Cooperative Formation of Icosahedral Proline Clusters from Dimers. Journal of the American Society for Mass Spectrometry, 2018, 29, 95-102.	2.8	3
144	Electrosynthesis of a Biaurone by Controlled Dimerization of Flavone: Mechanistic Insight and Large-Scale Application. Journal of Organic Chemistry, 2020, 85, 10658-10669.	3.2	3

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145	Singleâ€Cell Quantification of a Highly Biocompatible Dinuclear Iridium(III) Complex for Photocatalytic Cancer Therapy. Angewandte Chemie, 2022, 134, .	2.0	3
146	A Composite Energy Treatment for Sterically Hindered Cluster Models for the Si(100) Surface. Journal of Chemical Theory and Computation, 2012, 8, 5132-5136.	5.3	2
147	Modeling Nonperiodic Adsorption on Periodic Surfaces: A Composite Energy Approach for Low-Coverage Limits. Journal of Physical Chemistry C, 2012, 116, 12048-12054.	3.1	2
148	Hydroxyl Migration in Heterotrimetallic Clusters: An Assessment of Fluxionality Pathways. Journal of Physical Chemistry A, 2014, 118, 11047-11055.	2.5	2
149	Hidden complexities in the reaction of H2O2 and HNO revealed by ab initio quantum chemical investigations. Physical Chemistry Chemical Physics, 2017, 19, 29549-29560.	2.8	2
150	Untangling Hydrogen Bond Networks with Ion Mobility Spectrometry and Quantum Chemical Calculations: A Case Study on H⁺XPGG. Journal of Physical Chemistry B, 2019, 123, 5730-5741.	2.6	2
151	Exploring Reaction Energy Profiles Using the Molecules-in-Molecules Fragmentation-Based Approach. Journal of Chemical Theory and Computation, 2019, 15, 3991-4002.	5.3	2
152	Cluster Model Studies of Atomic Ordering in Group III Sublattice Growth over P-Rich InGaP₂(001) Surfaces. Journal of Physical Chemistry C, 2013, 117, 2078-2083.	3.1	0
153	Oxygen Activation by N-doped Graphitic Carbon Nanostructures. Materials Research Society Symposia Proceedings, 2015, 1725, 12.	0.1	0
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