Krishnan Raghavachari

List of Publications by Citations

149 papers	20,386 citations	41 h-index	142 g-index
158 ext. papers	21,677 ext. citations	5.9 avg, IF	6.72 L-index

#	Paper	IF	Citations
149	A fifth-order perturbation comparison of electron correlation theories. *Chemical Physics Letters*, **1989**, 157, 479-483	2.5	6685
148	Gaussian-3 (G3) theory for molecules containing first and second-row atoms. *Journal of Chemical Physics*, **1998**, 109, 7764-7776	3.9	2550
147	Assessment of Gaussian-2 and density functional theories for the computation of enthalpies of formation. *Journal of Chemical Physics*, **1997**, 106, 1063-1079	3.9	1822
146	Gaussian-4 theory. *Journal of Chemical Physics*, **2007**, 126, 084108	3.9	1466
145	Gaussian-3 theory using reduced Mo/ller-Plesset order. *Journal of Chemical Physics*, **1999**, 110, 4703-4709	3.9	1117
144	Assessment of Gaussian-3 and density functional theories for a larger experimental test set. *Journal of Chemical Physics*, **2000**, 112, 7374-7383	3.9	680
143	Gaussian-4 theory using reduced order perturbation theory. *Journal of Chemical Physics*, **2007**, 127, 124105	3.9	510
142	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	3.9	503
141	Gaussian-3X (G3X) theory: Use of improved geometries, zero-point energies, and Hartree□Fock basis sets. *Journal of Chemical Physics*, **2001**, 114, 108	3.9	454
140	Size-consistent Brueckner theory limited to double substitutions. *Chemical Physics Letters*, **1989**, 164, 185-192	2.5	440
139	Assessment of Gaussian-3 and density-functional theories on the G3/05 test set of experimental energies. *Journal of Chemical Physics*, **2005**, 123, 124107	3.9	297
138	Accurate Composite and Fragment-Based Quantum Chemical Models for Large Molecules. *Chemical Reviews*, **2015**, 115, 5643-77	68.1	169
137	Gn theory. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 810-825	7.9	159
136	Molecules-in-Molecules: An Extrapolated Fragment-Based Approach for Accurate Calculations on Large Molecules and Materials. *Journal of Chemical Theory and Computation*, **2011**, 7, 1336-43	6.4	143
135	Gaussian-2 theory: Use of higher level correlation methods, quadratic configuration interaction geometries, and second-order Mo/ller□lesset zero-point energies. *Journal of Chemical Physics*, **1995**, 103, 4192-4200	3.9	134
134	Gaussian-3 and related methods for accurate thermochemistry. *Theoretical Chemistry Accounts*, **2002**, 108, 61-70	1.9	115
133	Gaussian-3 theory using scaled energies. *Journal of Chemical Physics*, **2000**, 112, 1125-1132	3.9	111

132	Silicon Epoxide: Unexpected Intermediate during Silicon Oxide Formation. *Physical Review Letters*, **1998**, 81, 3908-3911	7.4	109
131	Anions Stabilize Each Other inside Macrocyclic Hosts. *Angewandte Chemie - International Edition*, **2016**, 55, 14057-14062	16.4	94
130	Role of interdimer interactions in NH3 dissociation on si(100)-(2x1). *Physical Review Letters*, **2001**, 86, 1046-9	7.4	91
129	Anion Binding in Solution: Beyond the Electrostatic Regime. *CheM*, **2017**, 3, 411-427	16.2	90
128	Aromatic and aliphatic CH hydrogen bonds fight for chloride while competing alongside ion pairing within triazolophanes. *Chemistry - A European Journal*, **2011**, 17, 312-21	4.8	90
127	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, 2669-75	6.4	88
126	Well-Defined Nanographene-Rhenium Complex as an Efficient Electrocatalyst and Photocatalyst for Selective CO Reduction. *Journal of the American Chemical Society*, **2017**, 139, 3934-3937	16.4	78
125	Structures of Mo2Oy- and Mo2Oy (y=2, 3, and 4) studied by anion photoelectron spectroscopy and density functional theory calculations. *Journal of Chemical Physics*, **2005**, 122, 094313	3.9	73
124	Chlorination of hydrogen-terminated silicon (111) surfaces. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **2005**, 23, 1100-1106	2.9	69
123	Insights into Working Principles of Ruthenium Polypyridyl Dye-Sensitized Solar Cells from First Principles Modeling. *Journal of Physical Chemistry C*, **2011**, 115, 4297-4306	3.8	64
122	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	16.4	64
121	Investigation of Gaussian4 theory for transition metal thermochemistry. *Journal of Physical Chemistry A*, **2009**, 113, 5170-5	2.8	62
120	The structure of n-alkanes: High precision ab initio calculation and relation to vibrational spectra. *Journal of Chemical Physics*, **1986**, 84, 6872-6878	3.9	60
119	Electrocatalytic oxygen activation by carbanion intermediates of nitrogen-doped graphitic carbon. *Journal of the American Chemical Society*, **2014**, 136, 3358-61	16.4	57
118	Two levels of conformational pre-organization consolidate strong CH hydrogen bonds in chloride-triazolophane complexes. *Chemical Communications*, **2011**, 47, 5979-81	5.8	57
117	Atomic Layer Deposition Growth Reactions of Al2O3 on Si(100)-2□. *Journal of Physical Chemistry B*, **2004**, 108, 4058-4062	3.4	56
116	Theoretical Thermochemistry for Organic Molecules: Development of the Generalized Connectivity-Based Hierarchy. *Journal of Chemical Theory and Computation*, **2011**, 7, 2094-103	6.4	55
115	Electrostatic and Allosteric Cooperativity in Ion-Pair Binding: A Quantitative and Coupled Experiment-Theory Study with Aryl-Triazole-Ether Macrocycles. *Journal of the American Chemical Society*, **2015**, 137, 9746-57	16.4	54

114	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	16.4	52
113	Atomic layer deposition of Al2O3 on H-passivated Si. I. Initial surface reaction pathways with H/Si(100)-2□1. *Journal of Chemical Physics*, **2003**, 118, 10221-10226	3.9	48
112	Strong CH...halide hydrogen bonds from 1,2,3-triazoles quantified using pre-organized and shape-persistent triazolophanes. *ChemPhysChem*, **2009**, 10, 2535-40	3.2	46
111	Flexibility Coexists with Shape-Persistence in Cyanostar Macrocycles. *Journal of the American Chemical Society*, **2016**, 138, 4843-4851	16.4	44
110	Extrapolation to the Gold-Standard in Quantum Chemistry: Computationally Efficient and Accurate CCSD(T) Energies for Large□Molecules Using an Automated Thermochemical Hierarchy. *Journal of Chemical Theory and Computation*, **2013**, 9, 3986-94	6.4	43
109	An overlooked yet ubiquitous fluoride congenitor: binding bifluoride in triazolophanes using computer-aided design. *Journal of the American Chemical Society*, **2014**, 136, 5078-89	16.4	41
108	Unusual products observed in gas-phase W(x)O(y)- + H2O and D2O reactions. *Journal of Chemical Physics*, **2009**, 130, 124314	3.9	41
107	Atomic layer deposition of Al2O3 on H-passivated Si: Al(CH3)2OH surface reactions with H/Si(100)□2□1. *Physical Review B*, **2003**, 68,	3.3	40
106	From atomic to molecular anions: a neutral receptor captures cyanide using strong C-H hydrogen bonds. *Chemistry - A European Journal*, **2011**, 17, 9123-9	4.8	39
105	Water reactivity with tungsten oxides: H(2) production and kinetic traps. *Journal of Chemical Physics* , **2009**, 131, 144302	3.9	39
104	Quantum chemical studies of semiconductor surface chemistry using cluster models. *Molecular Physics*, **2004**, 102, 381-393	1.7	39
103	Electronic structures of MoWO(y)- and MoWO(y) determined by anion photoelectron spectroscopy and DFT calculations. *Journal of Chemical Physics*, **2009**, 130, 124313	3.9	38
102	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, 17039-51	16.4	37
101	Addition of water to Al5O4- determined by anion photoelectron spectroscopy and quantum chemical calculations. *Journal of Chemical Physics*, **2005**, 122, 14313	3.9	37
100	Evaluation of Energy Gradients and Infrared Vibrational Spectra through Molecules-in-Molecules Fragment-Based Approach. *Journal of Chemical Theory and Computation*, **2015**, 11, 950-61	6.4	33
99	Vibrational Circular Dichroism Spectra for Large Molecules through Molecules-in-Molecules Fragment-Based Approach. *Journal of Chemical Theory and Computation*, **2015**, 11, 4238-47	6.4	30
98	Dimers of Dimers (DOD): A New Fragment-Based Method Applied to Large Water Clusters. *Journal of Chemical Theory and Computation*, **2014**, 10, 58-67	6.4	30
97	Connectivity-Based Hierarchy for theoretical thermochemistry: assessment using wave function-based methods. *Journal of Physical Chemistry A*, **2012**, 116, 7531-7	2.8	29

96	Hydrogen adsorption on phosphorus-rich (2□) indium phosphide (001). *Physical Review B*, **2002**, 65,	3.3	29
95	Termination of the W(2)O(y) (-)+H(2)O/D(2)O-->W(2)O(y+1) (-)+H(2)/D(2) sequential oxidation reaction: An exploration of kinetic versus thermodynamic effects. *Journal of Chemical Physics*, **2009**, 131, 144306	3.9	28
94	Importance of Steric Effects in Cluster Models of Silicon Surface Chemistry: ONIOM Studies of the Atomic Layer Deposition (ALD) of Al2O3 on H/Si(111)□ *Journal of Physical Chemistry A*, **2004**, 108, 2982-2987	2.8	28
93	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	6.4	26
92	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, 2012-23	6.4	26
91	Raman Optical Activity Spectra for Large Molecules through Molecules-in-Molecules Fragment-Based Approach. *Journal of Chemical Theory and Computation*, **2016**, 12, 585-94	6.4	26
90	Theoretical study of substituent effects on CH stretching frequencies. *Journal of Chemical Physics*, **1984**, 81, 2717-2722	3.9	24
89	Theoretical Study of Protein-Ligand Interactions Using the Molecules-in-Molecules Fragmentation-Based Method. *Journal of Chemical Theory and Computation*, **2018**, 14, 5143-5155	6.4	24
88	The successful merger of theoretical thermochemistry with fragment-based methods in quantum chemistry. *Accounts of Chemical Research*, **2014**, 47, 3596-604	24.3	23
87	Comparative study of water reactivity with Mo□(y)? and W□(y)? clusters: a combined experimental and theoretical investigation. *Journal of Chemical Physics*, **2014**, 141, 104310	3.9	23
86	Molybdenum oxides versus molybdenum sulfides: geometric and electronic structures of Mo□(y)? (X = O, S and y = 6, 9) clusters. *Journal of Physical Chemistry A*, **2011**, 115, 2291-6	2.8	23
85	In-vitro and In-vivo Photocatalytic Cancer Therapy with Biocompatible Iridium(III) Photocatalysts. *Angewandte Chemie - International Edition*, **2021**, 60, 9474-9479	16.4	23
84	Heats of Formation for CrO, CrO2, and CrO3: An Extreme Challenge for Black-Box Composite Procedures. *Journal of Chemical Theory and Computation*, **2012**, 8, 3159-66	6.4	22
83	Anions Stabilize Each Other inside Macrocyclic Hosts. *Angewandte Chemie*, **2016**, 128, 14263-14268	3.6	22
82	Assessment of Fragmentation Strategies for Large Proteins Using the Multilayer Molecules-in-Molecules Approach. *Journal of Chemical Theory and Computation*, **2018**, 14, 1383-1394	6.4	21
81	Application of the generalized connectivity-based hierarchy to biomonomers: enthalpies of formation of cysteine and methionine. *Journal of Physical Chemistry A*, **2013**, 117, 4973-80	2.8	20
80	Solving the Density Functional Conundrum: Elimination of Systematic Errors To Derive Accurate Reaction Enthalpies of Complex Organic Reactions. *Organic Letters*, **2017**, 19, 2576-2579	6.2	19
79	Hydrogen evolution from water through metal sulfide reactions. *Journal of Chemical Physics*, **2013**, 139, 204301	3.9	19

78	Host-Host Interactions Control Self-assembly and Switching of Triple and Double Decker Stacks of Tricarbazole Macrocycles Co-assembled with anti-Electrostatic Bisulfate Dimers. *Chemistry - A European Journal*, **2018**, 24, 9841-9852	4.8	18
77	C vs N: which end of the cyanide anion is a better hydrogen bond acceptor?. *Journal of Physical Chemistry A*, **2014**, 118, 7418-23	2.8	17
76	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	6.4	17
75	Infrared Intensities of (SiH) on H/Si(100)-2: Effect of O Incorporation and Agglomeration. *Journal of Physical Chemistry B*, **2004**, 108, 19388-19391	3.4	17
74	Energy Decomposition Analysis of Protein-Ligand Interactions Using Molecules-in-Molecules Fragmentation-Based Method. *Journal of Chemical Information and Modeling*, **2019**, 59, 3474-3484	6.1	16
73	Molecules-in-molecules fragment-based method for the evaluation of Raman spectra of large molecules. *Molecular Physics*, **2015**, 113, 3057-3066	1.7	16
72	Two methanes are better than one: a density functional theory study of the reactions of Mo2Oy- (y = 2-5) with methane. *Journal of Physical Chemistry A*, **2007**, 111, 8211-7	2.8	16
71	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 HNiCO, PdCO, and PtCO. *Journal of Chemical Physics*, **2003**, 119, 10591-10599	3.9	16
70	The microscopic origin of optical phonon evolution during water oxidation of Si(100). *Journal of Chemical Physics*, **2003**, 119, 2307-2313	3.9	16
69	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	6.4	15
68	Accurate p Evaluations for Complex Bio-Organic Molecules in Aqueous Media. *Journal of Chemical Theory and Computation*, **2019**, 15, 6025-6035	6.4	15
67	Prediction of Accurate Thermochemistry of Medium and Large Sized Radicals Using Connectivity-Based Hierarchy (CBH). *Journal of Chemical Theory and Computation*, **2014**, 10, 4342-50	6.4	15
66	Charge Transfer Across ONIOM QM:QM Boundaries: The Impact of Model System Preparation. *Journal of Chemical Theory and Computation*, **2010**, 6, 3131-6	6.4	15
65	Zero-Overlap Fluorophores for Fluorescent Studies at Any Concentration. *Journal of the American Chemical Society*, **2020**, 142, 12167-12180	16.4	14
64	Al5O4: A Superatom with Potential for New Materials Design. *Journal of Chemical Theory and Computation*, **2008**, 4, 2011-9	6.4	14
63	Insight into ethylene interactions with molybdenum suboxide cluster anions from photoelectron spectra of chemifragments. *Journal of Chemical Physics*, **2018**, 148, 054308	3.9	13
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61	Direct Reduction of Alkyl Monohalides at Silver in Dimethylformamide: Effects of Position and Identity of the Halogen. *ChemElectroChem*, **2015**, 2, 726-736	4.3	12

60	Basal Plane Fluorination of Graphene by XeF2 via a Radical Cation Mechanism. *Journal of Physical Chemistry Letters*, **2015**, 6, 3645-9	6.4	12
59	Anion-Binding Macrocycles Operate Beyond the Electrostatic Regime: Interaction Distances Matter. *Chemistry - A European Journal*, **2018**, 24, 14409-14417	4.8	12
58	The striking influence of oxophilicity differences in heterometallic Mo-Mn oxide cluster reactions with water. *Journal of Chemical Physics*, **2020**, 152, 054301	3.9	11
57	Restricted-Open-Shell G4(MP2)-Type Procedures. *Journal of Physical Chemistry A*, **2016**, 120, 9299-9304	2.8	11
56	Multi-state amine sensing by electron transfers in a BODIPY probe. *Organic and Biomolecular Chemistry*, **2020**, 18, 431-440	3.9	11
55	A Grotthuss-like proton shuttle in the anomalous CH carbocation: energetic and vibrational properties for isotopologues. *Physical Chemistry Chemical Physics*, **2016**, 18, 29395-29411	3.6	10
54	Reactions of Atomic Hydrogen with the Hydroxide- and Amine-Functionalized Si(100)-2□ Surfaces: Accurate Modeling of Hydrogen Abstraction Reactions Using Density Functional Theory. *Journal of Physical Chemistry C*, **2014**, 118, 8379-8386	3.8	10
53	Hydrogen evolution from water reactions with molybdenum sulfide cluster anions. *International Journal of Mass Spectrometry*, **2018**, 434, 193-201	1.9	10
52	Accurate and computationally efficient prediction of thermochemical properties of biomolecules using the generalized connectivity-based hierarchy. *Journal of Physical Chemistry B*, **2014**, 118, 9631-43	3.4	9
51	Role of weakly bound complexes in temperature-dependence and relative rates of M(x)O(y)(-) + H2O (M = Mo, W) reactions. *Journal of Chemical Physics*, **2016**, 144, 074307	3.9	9
50	Molybdenum Oxide Cluster Anion Reactions with CH and HO: Cooperativity and Chemifragmentation. *Journal of Physical Chemistry A*, **2018**, 122, 41-52	2.8	8
49	Redox "Innocence" of Re(I) in Electrochemical CO Reduction Catalyzed by Nanographene-Re Complexes. *Inorganic Chemistry*, **2018**, 57, 10548-10556	5.1	8
48	Multiple Solutions to the Single-Reference CCSD Equations for NiH. *Journal of Chemical Theory and Computation*, **2010**, 6, 2714-20	6.4	8
47	Interaction of Lewis Acids with Si(100)-2□ and Ge(100)-2□ Surfaces. *Journal of Physical Chemistry C*, **2009**, 113, 10146-10150	3.8	8
46	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	6.4	8
45	In-vitro and In-vivo Photocatalytic Cancer Therapy with Biocompatible Iridium(III) Photocatalysts. *Angewandte Chemie*, **2021**, 133, 9560-9565	3.6	8
44	Applications of isodesmic-type reactions for computational thermochemistry. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1501	7.9	8
43	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	6.4	8

42	Amphiphile self-assembly dynamics at the solution-solid interface reveal asymmetry in head/tail desorption. *Chemical Communications*, **2018**, 54, 10076-10079	5.8	7
41	Electrostatic Potential-Based Method of Balancing Charge Transfer Across ONIOM QM:QM Boundaries. *Journal of Chemical Theory and Computation*, **2014**, 10, 4351-9	6.4	7
40	Extending Molecular Lines on the Si(100)-2 × 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	6.4	7
39	Hydrogen evolution from water using Mo-oxide clusters in the gas phase: DFT modeling of a complete catalytic cycle using a MoO/MoO cluster couple. *Physical Chemistry Chemical Physics*, **2016**, 18, 25687-25692	3.6	7
38	Line Growth on the H/Si(100)-2 × 1 Surface: Density Functional Study of Allylic Mercaptan Reaction Mechanisms. *Journal of Physical Chemistry C*, **2009**, 113, 18817-18822	3.8	6
37	Phosphine adsorption on the In-rich InP(001) surface: evidence of surface dative bonds at room temperature. *Langmuir*, **2007**, 23, 10109-15	4	6
36	Bond Activation and Hydrogen Evolution from Water through Reactions with MS (M = Mo, W) and WS Anionic Clusters. *Journal of Physical Chemistry A*, **2017**, 121, 1760-1767	2.8	5
35	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	2.8	5
34	Solution-Mediated Annealing Pathways Are Critical for Supramolecular Ordering of Complex Macrocycles at Surfaces. *Journal of Physical Chemistry C*, **2020**, 124, 6689-6699	3.8	5
33	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	6.4	5
32	H2S Reactivity on Oxygen-Deficient Heterotrimetallic Cores: Cluster Fluxionality Simulates Dynamic Aspects of Surface Chemical Reactions. *Journal of Physical Chemistry A*, **2016**, 120, 466-72	2.8	5
31	Mo Insertion into the H Bond in MoS + H Reactions. *Journal of Physical Chemistry A*, **2019**, 123, 7261-7269	2.8	5
30	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	3.6	5
29	Electronic Energies Are Not Enough: An Ion Mobility-Aided, Quantum Chemical Benchmark Analysis of HGPGG Conformers. *Journal of Chemical Theory and Computation*, **2018**, 14, 5406-5418	6.4	5
28	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	6.1	4
27	Accurate Thermochemistry for Organic Cations via Error Cancellation using Connectivity-Based Hierarchy. *Journal of Physical Chemistry A*, **2018**, 122, 1807-1812	2.8	4
26	Molecules-in-Molecules Fragment-Based Method for the Accurate Evaluation of Vibrational and Chiroptical Spectra for Large Molecules **2017**, 141-163		4
25	Electronic structures and water reactivity of mixed metal sulfide cluster anions. *Journal of Chemical Physics*, **2014**, 141, 074305	3.9	4

24	Predicting PH vibrations of gas phase molecules and surface-adsorbed species using bond length-frequency correlations. *Journal of Computational Chemistry*, **2009**, 30, 1872-81	3.5	4
23	In-Rich Surface Growth on P-Rich InP(001) (2 □) Surface: Structural and Mechanistic Study. *Journal of Physical Chemistry C*, **2008**, 112, 6022-6026	3.8	4
22	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	3.8	3
21	Mechanistic Role of Two-State Reactivity in a Molecular MoS Edge-Site Analogue for Hydrogen Evolution Electrocatalysis. *Inorganic Chemistry*, **2018**, 57, 9167-9174	5.1	3
20	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	3.8	3
19	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	6.4	3
18	G4 accuracy at DFT cost: unlocking accurate redox potentials for organic molecules using systematic error cancellation. *Physical Chemistry Chemical Physics*, **2020**, 22, 4439-4452	3.6	3
17	Breaking a bottleneck: Accurate extrapolation to "gold standard" CCSD(T) energies for large open shell organic radicals at reduced computational cost. *Journal of Computational Chemistry*, **2016**, 37, 286-95	3.5	3
16	Hidden complexities in the reaction of HO and HNO revealed by ab initio quantum chemical investigations. *Physical Chemistry Chemical Physics*, **2017**, 19, 29549-29560	3.6	2
15	A Composite Energy Treatment for Sterically Hindered Cluster Models for the Si(100) Surface. *Journal of Chemical Theory and Computation*, **2012**, 8, 5132-6	6.4	2
14	Modeling Nonperiodic Adsorption on Periodic Surfaces: A Composite Energy Approach for Low-Coverage Limits. *Journal of Physical Chemistry C*, **2012**, 116, 12048-12054	3.8	2
13	Highly Efficient Ir(III)-Coumarin Photo-Redox Catalyst for Synergetic Multi-Mode Cancer Photo-Therapy. *Chemistry - A European Journal*, **2021**,	4.8	2
12	Cooperative Formation of Icosahedral Proline Clusters from Dimers. *Journal of the American Society for Mass Spectrometry*, **2018**, 29, 95-102	3.5	2
11	Untangling Hydrogen Bond Networks with Ion Mobility Spectrometry and Quantum Chemical Calculations: A Case Study on HXPGG. *Journal of Physical Chemistry B*, **2019**, 123, 5730-5741	3.4	1
10	Hydroxyl migration in heterotrimetallic clusters: an assessment of fluxionality pathways. *Journal of Physical Chemistry A*, **2014**, 118, 11047-55	2.8	1
9	Charge redistribution in QM:QM ONIOM model systems: a constrained density functional theory approach. *Molecular Physics*, **2017**, 115, 2813-2822	1.7	1
8	A Fragmentation-Based Graph Embedding Framework for QM/ML. *Journal of Physical Chemistry A*, **2021**, 125, 6872-6880	2.8	1
7	Photosensitized [2+2]-Cycloadditions of Alkenylboronates and Alkenes.. *Angewandte Chemie - International Edition*, **2022**, e202200725	16.4	1

6	Electrosynthesis of a Biaurone by Controlled Dimerization of Flavone: Mechanistic Insight and Large-Scale Application. *Journal of Organic Chemistry*, **2020**, 85, 10658-10669	4.2	0
5	Electrostatically embedded molecules-in-molecules approach and its application to molecular clusters. *Journal of Computational Chemistry*, **2021**, 42, 719-734	3.5	0
4	Exploring Reaction Energy Profiles Using the Molecules-in-Molecules Fragmentation-Based Approach. *Journal of Chemical Theory and Computation*, **2019**, 15, 3991-4002	6.4	
3	Oxygen Activation by N-doped Graphitic Carbon Nanostructures. *Materials Research Society Symposia Proceedings*, **2015**, 1725, 12		
2	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	3.8	
1	Interaction-Deletion: A Composite Energy Method for the Optimization of Molecular Systems Selectively Removing Specific Nonbonded Interactions. *Journal of Physical Chemistry A*, **2021**, 125, 4668-4682	2.8	