Krishnan Raghavachari

List of Publications by Year
in descending order

154 papers	23,177 citations	71004 43 h-index	8627 151 g-index
158 all docs	158 docs citations	158 times ranked	12629 citing authors

#	Article	IF	Citations
1	Highly Efficient Ir(III)â€Coumarin Photoâ€Redox Catalyst for Synergetic Multiâ€Mode Cancer Photoâ€Therapy. Chemistry - A European Journal, 2022, 28, .	1.7	11
2	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.	6.6	22
3	Three-Dimensional Convolutional Neural Networks Utilizing Molecular Topological Features for Accurate Atomization Energy Predictions. Journal of Chemical Theory and Computation, 2022, 18, 2132-2143.	2.3	4
4	Singleâ€Cell Quantification of a Highly Biocompatible Dinuclear Iridium(III) Complex for Photocatalytic Cancer Therapy. Angewandte Chemie, 2022, 134, .	1.6	3
5	Singleâ€Cell Quantification of a Highly Biocompatible Dinuclear Iridium(III) Complex for Photocatalytic Cancer Therapy. Angewandte Chemie - International Edition, 2022, 61, .	7.2	22
6	Photosensitized [2+2]â€Cycloadditions of Alkenylboronates and Alkenes. Angewandte Chemie - International Edition, 2022, 61, e202200725.	7.2	22
7	Photosensitized [2+2]â€Cycloadditions of Alkenylboronates and Alkenes. Angewandte Chemie, 2022, 134, .	1.6	7
8	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.	1.3	5
9	Applications of isodesmicâ€type reactions for computational thermochemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1501.	6.2	25
10	Electrostatically embedded moleculesâ€inâ€molecules approach and its application to molecular clusters. Journal of Computational Chemistry, 2021, 42, 719-734.	1.5	4
11	Inâ€vitro and Inâ€vivo Photocatalytic Cancer Therapy with Biocompatible Iridium(III) Photocatalysts. Angewandte Chemie - International Edition, 2021, 60, 9474-9479.	7.2	89
12	Inâ€vitro and Inâ€vivo Photocatalytic Cancer Therapy with Biocompatible Iridium(III) Photocatalysts. Angewandte Chemie, 2021, 133, 9560-9565.	1.6	24
13	Interactionâ€“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.	1.1	0
14	A Fragmentation-Based Graph Embedding Framework for QM/ML. Journal of Physical Chemistry A, 2021, 125, 6872-6880.	1.1	9
15	Multi-state amine sensing by electron transfers in a BODIPY probe. Organic and Biomolecular Chemistry, 2020, 18, 431-440.	1.5	19
16	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.	2.3	18
17	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.	1.3	19
18	Electrosynthesis of a Biaurone by Controlled Dimerization of Flavone: Mechanistic Insight and Large-Scale Application. Journal of Organic Chemistry, 2020, 85, 10658-10669.	1.7	3

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19	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.	2.5	9
20	Zero-Overlap Fluorophores for Fluorescent Studies at Any Concentration. Journal of the American Chemical Society, 2020, 142, 12167-12180.	6.6	30
21	Solution-Mediated Annealing Pathways Are Critical for Supramolecular Ordering of Complex Macrocycles at Surfaces. Journal of Physical Chemistry C, 2020, 124, 6689-6699.	1.5	7
22	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.	2.3	7
23	The striking influence of oxophilicity differences in heterometallic Moâ€“Mn oxide cluster reactions with water. Journal of Chemical Physics, 2020, 152, 054301.	1.2	15
24	G4 accuracy at DFT cost: unlocking accurate redox potentials for organic molecules using systematic error cancellation. Physical Chemistry Chemical Physics, 2020, 22, 4439-4452.	1.3	13
25	Mo Insertion into the H₂ Bond in Mo_xS_y^{â€“} + H₂ Reactions. Journal of Physical Chemistry A, 2019, 123, 7261-7269.	1.1	7
26	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.	1.5	6
27	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.	2.3	34
28	Energy Decomposition Analysis of Proteinâ€“Ligand Interactions Using Molecules-in-Molecules Fragmentation-Based Method. Journal of Chemical Information and Modeling, 2019, 59, 3474-3484.	2.5	35
29	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.	1.2	2
30	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.	2.3	6
31	Accurate pK_a Evaluations for Complex Bio-Organic Molecules in Aqueous Media. Journal of Chemical Theory and Computation, 2019, 15, 6025-6035.	2.3	31
32	Exploring Reaction Energy Profiles Using the Molecules-in-Molecules Fragmentation-Based Approach. Journal of Chemical Theory and Computation, 2019, 15, 3991-4002.	2.3	2
33	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.	1.1	14
34	Insight into ethylene interactions with molybdenum suboxide cluster anions from photoelectron spectra of chemifragments. Journal of Chemical Physics, 2018, 148, 054308.	1.2	17
35	Assessment of Fragmentation Strategies for Large Proteins Using the Multilayer Molecules-in-Molecules Approach. Journal of Chemical Theory and Computation, 2018, 14, 1383-1394.	2.3	29
36	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.	1.7	24

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37	Accurate Thermochemistry for Organic Cations via Error Cancellation using Connectivity-Based Hierarchy. Journal of Physical Chemistry A, 2018, 122, 1807-1812.	1.1	12
38	Molybdenum Oxide Cluster Anion Reactions with C₂H₄ and H₂O: Cooperativity and Chemifragmentation. Journal of Physical Chemistry A, 2018, 122, 41-52.	1.1	10
39	Cooperative Formation of Icosahedral Proline Clusters from Dimers. Journal of the American Society for Mass Spectrometry, 2018, 29, 95-102.	1.2	3
40	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.	2.3	12
41	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.	6.6	90
42	Theoretical Study of Proteinâ€“Ligand Interactions Using the Molecules-in-Molecules Fragmentation-Based Method. Journal of Chemical Theory and Computation, 2018, 14, 5143-5155.	2.3	33
43	Hydrogen evolution from water reactions with molybdenum sulfide cluster anions. International Journal of Mass Spectrometry, 2018, 434, 193-201.	0.7	14
44	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.	2.3	7
45	Amphiphile self-assembly dynamics at the solution-solid interface reveal asymmetry in head/tail desorption. Chemical Communications, 2018, 54, 10076-10079.	2.2	8
46	Anionâ€Binding Macrocycles Operate Beyond the Electrostatic Regime: Interaction Distances Matter. Chemistry - A European Journal, 2018, 24, 14409-14417.	1.7	20
47	Mechanistic Role of Two-State Reactivity in a Molecular MoS₂ Edge-Site Analogue for Hydrogen Evolution Electrocatalysis. Inorganic Chemistry, 2018, 57, 9167-9174.	1.9	4
48	Redox â€œInnocenceâ€•of Re(I) in Electrochemical CO2 Reduction Catalyzed by Nanographeneâ€“Re Complexes. Inorganic Chemistry, 2018, 57, 10548-10556.	1.9	11
49	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.	1.1	6
50	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.	6.6	95
51	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.	2.3	40
52	Solving the Density Functional Conundrum: Elimination of Systematic Errors To Derive Accurate Reaction Enthalpies of Complex Organic Reactions. Organic Letters, 2017, 19, 2576-2579.	2.4	27
53	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.	1.5	3
54	Hidden complexities in the reaction of H2O2 and HNO revealed by ab initio quantum chemical investigations. Physical Chemistry Chemical Physics, 2017, 19, 29549-29560.	1.3	2

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55	Anion Binding in Solution: Beyond the Electrostatic Regime. CheM, 2017, 3, 411-427.	5.8	129
56	Charge redistribution in QM:QM ONIOM model systems: a constrained density functional theory approach. Molecular Physics, 2017, 115, 2813-2822.	0.8	4
57	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.	1.5	6
58	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.	1.3	15
59	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.	1.2	11
60	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.	1.3	9
61	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.	6.6	88
62	Anions Stabilize Each Other inside Macrocyclic Hosts. Angewandte Chemie, 2016, 128, 14263-14268.	1.6	25
63	Anions Stabilize Each Other inside Macrocyclic Hosts. Angewandte Chemie - International Edition, 2016, 55, 14057-14062.	7.2	115
64	A Grotthuss-like proton shuttle in the anomalous C₂H₃⁺carbocation: energetic and vibrational properties for isotopologues. Physical Chemistry Chemical Physics, 2016, 18, 29395-29411.	1.3	11
65	Restricted-Open-Shell G4(MP2)-Type Procedures. Journal of Physical Chemistry A, 2016, 120, 9299-9304.	1.1	19
66	Raman Optical Activity Spectra for Large Molecules through Molecules-in-Molecules Fragment-Based Approach. Journal of Chemical Theory and Computation, 2016, 12, 585-594.	2.3	32
67	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.	1.1	8
68	Flexibility Coexists with Shape-Persistence in Cyanostar Macrocycles. Journal of the American Chemical Society, 2016, 138, 4843-4851.	6.6	53
69	Molecules-in-molecules fragment-based method for the evaluation of Raman spectra of large molecules. Molecular Physics, 2015, 113, 3057-3066.	0.8	22
70	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.	2.3	39
71	Direct Reduction of Alkyl Monohalides at Silver in Dimethylformamide: Effects of Position and Identity of the Halogen. ChemElectroChem, 2015, 2, 726-736.	1.7	13
72	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.	6.6	69

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73	Oxygen Activation by N-doped Graphitic Carbon Nanostructures. Materials Research Society Symposia Proceedings, 2015, 1725, 12.	0.1	0
74	Accurate Composite and Fragment-Based Quantum Chemical Models for Large Molecules. Chemical Reviews, 2015, 115, 5643-5677.	23.0	225
75	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.	2.3	34
76	Vibrational Circular Dichroism Spectra for Large Molecules through Molecules-in-Molecules Fragment-Based Approach. Journal of Chemical Theory and Computation, 2015, 11, 4238-4247.	2.3	40
77	Basal Plane Fluorination of Graphene by XeF₂ via a Radical Cation Mechanism. Journal of Physical Chemistry Letters, 2015, 6, 3645-3649.	2.1	14
78	Comparative study of water reactivity with Mo2Oyâ^' and W2Oyâ^' clusters: A combined experimental and theoretical investigation. Journal of Chemical Physics, 2014, 141, 104310.	1.2	28
79	Electronic structures and water reactivity of mixed metal sulfide cluster anions. Journal of Chemical Physics, 2014, 141, 074305.	1.2	5
80	An Overlooked yet Ubiquitous Fluoride Congenitor: Binding Bifluoride in Triazolophanes Using Computer-Aided Design. Journal of the American Chemical Society, 2014, 136, 5078-5089.	6.6	47
81	Hydroxyl Migration in Heterotrimetallic Clusters: An Assessment of Fluxionality Pathways. Journal of Physical Chemistry A, 2014, 118, 11047-11055.	1.1	2
82	The Successful Merger of Theoretical Thermochemistry with Fragment-Based Methods in Quantum Chemistry. Accounts of Chemical Research, 2014, 47, 3596-3604.	7.6	34
83	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.	2.3	30
84	Dimers of Dimers (DOD): A New Fragment-Based Method Applied to Large Water Clusters. Journal of Chemical Theory and Computation, 2014, 10, 58-67.	2.3	33
85	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.	1.5	10
86	Electrocatalytic Oxygen Activation by Carbanion Intermediates of Nitrogen-Doped Graphitic Carbon. Journal of the American Chemical Society, 2014, 136, 3358-3361.	6.6	68
87	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.	1.2	13
88	Electrostatic Potential-Based Method of Balancing Charge Transfer Across ONIOM QM:QM Boundaries. Journal of Chemical Theory and Computation, 2014, 10, 4351-4359.	2.3	8
89	C vs N: Which End of the Cyanide Anion Is a Better Hydrogen Bond Acceptor?. Journal of Physical Chemistry A, 2014, 118, 7418-7423.	1.1	22
90	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.	2.3	64

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91	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.	6.6	41
92	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.	1.5	0
93	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.	1.1	27
94	Hydrogen evolution from water through metal sulfide reactions. Journal of Chemical Physics, 2013, 139, 204301.	1.2	23
95	A Composite Energy Treatment for Sterically Hindered Cluster Models for the Si(100) Surface. Journal of Chemical Theory and Computation, 2012, 8, 5132-5136.	2.3	2
96	Modeling Nonperiodic Adsorption on Periodic Surfaces: A Composite Energy Approach for Low-Coverage Limits. Journal of Physical Chemistry C, 2012, 116, 12048-12054.	1.5	2
97	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.	2.3	104
98	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.	2.3	26
99	Connectivity-Based Hierarchy for Theoretical Thermochemistry: Assessment Using Wave Function-Based Methods. Journal of Physical Chemistry A, 2012, 116, 7531-7537.	1.1	41
100	Two levels of conformational pre-organization consolidate strong CH hydrogen bonds in chlorideâ€“triazolophane complexes. Chemical Communications, 2011, 47, 5979.	2.2	60
101	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.	1.1	28
102	Theoretical Thermochemistry for Organic Molecules: Development of the Generalized Connectivity-Based Hierarchy. Journal of Chemical Theory and Computation, 2011, 7, 2094-2103.	2.3	77
103	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.	2.3	177
104	Insights into Working Principles of Ruthenium Polypyridyl Dye-Sensitized Solar Cells from First Principles Modeling. Journal of Physical Chemistry C, 2011, 115, 4297-4306.	1.5	71
105	Gn theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 810-825.	6.2	189
106	Aromatic and Aliphatic CH Hydrogen Bonds Fight for Chloride while Competing Alongside Ion Pairing within Triazolophanes. Chemistry - A European Journal, 2011, 17, 312-321.	1.7	98
107	From Atomic to Molecular Anions: A Neutral Receptor Captures Cyanide Using Strong Cï£¿H Hydrogen Bonds. Chemistry - A European Journal, 2011, 17, 9123-9129.	1.7	41
108	Multiple Solutions to the Single-Reference CCSD Equations for NiH. Journal of Chemical Theory and Computation, 2010, 6, 2714-2720.	2.3	14

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109	Charge Transfer Across ONIOM QM:QM Boundaries: The Impact of Model System Preparation. Journal of Chemical Theory and Computation, 2010, 6, 3131-3136.	2.3	18
110	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.	2.1	19
111	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.	2.1	8
112	Water reactivity with tungsten oxides: H2 production and kinetic traps. Journal of Chemical Physics, 2009, 131, 144302.	1.2	39
113	Unusual products observed in gas-phase WxOyâ^'+H2O and D2O reactions. Journal of Chemical Physics, 2009, 130, 124314.	1.2	42
114	Electronic structures of MoWOyâ^' and MoWOy determined by anion photoelectron spectroscopy and DFT calculations. Journal of Chemical Physics, 2009, 130, 124313.	1.2	39
115	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.	1.2	29
116	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.	1.0	50
117	Predicting PH vibrations of gas phase molecules and surfaceâ€adsorbed species using bond lengthâ€frequency correlations. Journal of Computational Chemistry, 2009, 30, 1872-1881.	1.5	4
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.	1.5	8
119	Investigation of Gaussian4 Theory for Transition Metal Thermochemistry. Journal of Physical Chemistry A, 2009, 113, 5170-5175.	1.1	65
120	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.	1.5	7
121	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.	1.5	5
122	Al5O4: A Superatom with Potential for New Materials Design. Journal of Chemical Theory and Computation, 2008, 4, 2011-2019.	2.3	14
123	Phosphine Adsorption on the In-Rich InP(001) Surface:â€‰ Evidence of Surface Dative Bonds at Room Temperature. Langmuir, 2007, 23, 10109-10115.	1.6	7
124	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.	1.1	17
125	Gaussian-4 theory using reduced order perturbation theory. Journal of Chemical Physics, 2007, 127, 124105.	1.2	598
126	Gaussian-4 theory. Journal of Chemical Physics, 2007, 126, 084108.	1.2	1,741

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127	Assessment of Gaussian-3 and density-functional theories on the G3/05 test set of experimental energies. Journal of Chemical Physics, 2005, 123, 124107.	1.2	320
128	Chlorination of hydrogen-terminated silicon (111) surfaces. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2005, 23, 1100-1106.	0.9	71
129	Addition of water to Al5O4â^' determined by anion photoelectron spectroscopy and quantum chemical calculations. Journal of Chemical Physics, 2005, 122, 014313.	1.2	37
130	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.	1.2	75
131	Quantum chemical studies of semiconductor surface chemistry using cluster models. Molecular Physics, 2004, 102, 381-393.	0.8	43
132	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.	1.1	29
133	Atomic Layer Deposition Growth Reactions of Al2O3 on Si(100)-2Ã—1. Journal of Physical Chemistry B, 2004, 108, 4058-4062.	1.2	60
134	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.	1.2	17
135	Atomic layer deposition ofAl2O3on H-passivated Si:â€ƒAl(CH3)2OHsurface reactions withH/Si(100)â^'2Ã—1. Physical Review B, 2003, 68, .	1.1	41
136	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.	1.2	16
137	The microscopic origin of optical phonon evolution during water oxidation of Si(100). Journal of Chemical Physics, 2003, 119, 2307-2313.	1.2	16
138	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.	1.2	51
139	Hydrogen adsorption on phosphorus-rich(2Ã—1)indium phosphide (001). Physical Review B, 2002, 65, .	1.1	29
140	Gaussian-3 and related methods for accurate thermochemistry. Theoretical Chemistry Accounts, 2002, 108, 61-70.	0.5	122
141	Gaussian-3X (G3X) theory: Use of improved geometries, zero-point energies, and Hartreeâ€“Fock basis sets. Journal of Chemical Physics, 2001, 114, 108.	1.2	477
142	Role of Interdimer Interactions inNH3Dissociation onSi(100)â^'(2Ã—1). Physical Review Letters, 2001, 86, 1046-1049.	2.9	96
143	Gaussian-3 theory using scaled energies. Journal of Chemical Physics, 2000, 112, 1125-1132.	1.2	119
144	Assessment of Gaussian-3 and density functional theories for a larger experimental test set. Journal of Chemical Physics, 2000, 112, 7374-7383.	1.2	711

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145	Gaussian-3 theory using reduced Mo/ller-Plesset order. Journal of Chemical Physics, 1999, 110, 4703-4709.	1.2	1,201
146	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.	1.2	536
147	Gaussian-3 (G3) theory for molecules containing first and second-row atoms. Journal of Chemical Physics, 1998, 109, 7764-7776.	1.2	2,746
148	Silicon Epoxide: Unexpected Intermediate during Silicon Oxide Formation. Physical Review Letters, 1998, 81, 3908-3911.	2.9	112
149	Assessment of Gaussian-2 and density functional theories for the computation of enthalpies of formation. Journal of Chemical Physics, 1997, 106, 1063-1079.	1.2	2,015
150	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.	1.2	146
151	Size-consistent Brueckner theory limited to double substitutions. Chemical Physics Letters, 1989, 164, 185-192.	1.2	478
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