

Kenneth D Jordan

List of Publications by Year in descending order

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135
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135
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135
times ranked

5423
citing authors

#	ARTICLE	IF	CITATIONS
1	Spectral Signatures of Hydrated Proton Vibrations in Water Clusters. <i>Science</i> , 2005, 308, 1765-1769.	12.6	712
2	Infrared Spectrum of a Molecular Ice Cube: The S4 and D2d Water Octamers in Benzene-(Water) ₈ . <i>Science</i> , 1997, 276, 1678-1681.	12.6	433
3	Studies of the temporary anion states of unsaturated hydrocarbons by electron transmission spectroscopy. <i>Accounts of Chemical Research</i> , 1978, 11, 341-348.	15.6	425
4	Ab initio electronic structure of anions. <i>Chemical Reviews</i> , 1987, 87, 535-555.	47.7	336
5	Temporary anion states of polyatomic hydrocarbons. <i>Chemical Reviews</i> , 1987, 87, 557-588.	47.7	334
6	THEORY OF DIPOLE-BOUND ANIONS. <i>Annual Review of Physical Chemistry</i> , 2003, 54, 367-396.	10.8	273
7	Theoretical Study of Oxygen Adsorption on Graphite and the (8,0) Single-walled Carbon Nanotube. <i>Journal of Physical Chemistry B</i> , 2001, 105, 11227-11232.	2.6	258
8	Wet Electrons at the H ₂ O/TiO ₂ (110) Surface. <i>Science</i> , 2005, 308, 1154-1158.	12.6	239
9	Spectroscopic snapshots of the proton-transfer mechanism in water. <i>Science</i> , 2016, 354, 1131-1135.	12.6	213
10	Theoretical Characterization of the Structures and Vibrational Spectra of Benzene ⁺ (H ₂ O) _n (n = 1-3) Clusters. <i>The Journal of Physical Chemistry</i> , 1996, 100, 7810-7821.	2.9	187
11	Contribution of electron correlation to the stability of dipole-bound anionic states. <i>Physical Review A</i> , 1996, 54, 1906-1909.	2.5	167
12	Electronic Structure of Dipole-Bound Anions. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2624-2633.	2.5	148
13	Resonant ion-dip infrared spectroscopy of the S4 and D2d water octamers in benzene-(water) ₈ and benzene ₂ -(water) ₈ . <i>Journal of Chemical Physics</i> , 1998, 109, 6601-6614.	3.0	123
14	Calculation of the Si-H bond energies for the monohydride phase of Si(100). <i>Journal of Chemical Physics</i> , 1991, 95, 8652-8654.	3.0	116
15	Infrared spectroscopy of negatively charged water clusters: Evidence for a linear network. <i>Journal of Chemical Physics</i> , 1999, 110, 6268-6277.	3.0	116
16	An Assessment of the vdW-TS Method for Extended Systems. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1503-1513.	5.3	112
17	Benchmark calculations of water-graphene interaction energies: Extrapolation to the water-graphene limit and assessment of dispersion-corrected DFT methods. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6375.	2.8	111
18	Snapshots of Proton Accommodation at a Microscopic Water Surface: Understanding the Vibrational Spectral Signatures of the Charge Defect in Cryogenically Cooled H ⁺ (H ₂ O) _n Clusters. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9425-9440.	2.5	111

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19	CO ₂ ~Fluorocarbon and CO ₂ ~Hydrocarbon Interactions from First-Principles Calculations. Journal of Physical Chemistry A, 1998, 102, 2231-2236.	2.5	107
20	A second generation distributed point polarizable water model. Journal of Chemical Physics, 2010, 132, 014309.	3.0	106
21	How the Shape of an H-Bonded Network Controls Proton-Coupled Water Activation in HONO Formation. Science, 2010, 327, 308-312.	12.6	99
22	Electron Binding Motifs of (H ₂ O) _n -Clusters. Journal of the American Chemical Society, 2006, 128, 5828-5833.	13.7	94
23	Energies of dipole-bound anionic states. International Journal of Quantum Chemistry, 1997, 64, 183-191.	2.0	86
24	Theoretical Characterization of the (H ₂ O) ₂₁ Cluster: Application of ann-body Decomposition Procedure. Journal of Physical Chemistry B, 2006, 110, 18872-18878.	2.6	84
25	Resonant ion-dip infrared spectroscopy of benzene~(water) ₉ : Expanding the cube. Journal of Chemical Physics, 2000, 113, 2290-2303.	3.0	81
26	Assignments of the temporary anion states of the chloromethanes. The Journal of Physical Chemistry, 1990, 94, 5666-5669.	2.9	80
27	QMCPACK: Advances in the development, efficiency, and application of auxiliary field and real-space variational and diffusion quantum Monte Carlo. Journal of Chemical Physics, 2020, 152, 174105.	3.0	80
28	Dipole-bound anions of carbonyl, nitrile, and sulfoxide containing molecules. Journal of Chemical Physics, 2003, 119, 3650-3660.	3.0	79
29	DF-DFT-SAPT Investigation of the Interaction of a Water Molecule to Coronene and Dodecabenzocoronene: Implications for the Water~Graphite Interaction. Journal of Physical Chemistry C, 2009, 113, 10242-10248.	3.1	79
30	Fluorescence~dip infrared spectroscopy of tropolone and tropolone~OD. Journal of Chemical Physics, 1996, 105, 2595-2604.	3.0	75
31	Existence of a Correlation Bound <i>s</i> -Type Anion State of C ₆₀ . Journal of Physical Chemistry Letters, 2013, 4, 849-853.	4.6	71
32	CHEMISTRY: A Fresh Look at Electron Hydration. Science, 2004, 306, 618-619.	12.6	70
33	Model Potential Approaches for Describing the Interaction of Excess Electrons with Water Clusters: Incorporation of Long-Range Correlation Effects. Journal of Physical Chemistry A, 2008, 112, 11021-11035.	2.5	68
34	Molecular visualization in chemistry education: the role of multidisciplinary collaboration. Chemistry Education Research and Practice, 2005, 6, 136-149.	2.5	66
35	Parallel-Tempering Monte Carlo Study of (H ₂ O) _{n=6-9} . Journal of Physical Chemistry A, 2003, 107, 7380-7389.	2.5	65
36	Dipole-bound anions of highly polar molecules: Ethylene carbonate and vinylene carbonate. Journal of Chemical Physics, 2004, 120, 685-690.	3.0	63

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37	Large anharmonic effects in the infrared spectra of the symmetrical CH ₃ NO ₂ ⁺ ⋯(H ₂ O) and CH ₃ CO ₂ ⁻ ⋯(H ₂ O) complexes. <i>Journal of Chemical Physics</i> , 2003, 119, 10138-10145.	3.0	57
38	Comment on the structure and stability of (CO ₂) ₂ . <i>Journal of Chemical Physics</i> , 1979, 70, 4422-4424.	3.0	56
39	Quantum Drude Oscillator Model for Describing the Interaction of Excess Electrons with Water Clusters: An Application to (H ₂ O) ₁₃ . <i>Journal of Physical Chemistry A</i> , 2005, 109, 11531-11538.	2.5	54
40	Assessment of Various Electronic Structure Methods for Characterizing Temporary Anion States: Application to the Ground State Anions of N ₂ , C ₂ H ₂ , C ₂ H ₄ , and C ₆ H ₆ . <i>Journal of Physical Chemistry A</i> , 2014, 118, 7489-7497.	2.5	52
41	Nonvalence Correlation-Bound Anion State of C ₆ F ₆ : Doorway to Low-Energy Electron Capture. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7201-7205.	2.5	51
42	Interplay between hydrogen bonding and electron solvation on hydrated TiO ₂ (110). <i>Physical Review B</i> , 2006, 73, .	3.2	50
43	Negative electron affinities from conventional electronic structure methods. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	1.4	50
44	Unraveling the Anomalous Solvatochromic Response of the Formate Ion Vibrational Spectrum: An Infrared, Ar-Tagging Study of the HCO ₂ ⁻ , DCO ₂ ⁻ , and HCO ₂ ⁻ ⋯H ₂ O Ions. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2437-2441.	4.6	49
45	Theoretical studies of positron-molecule complexes. <i>Journal of Chemical Physics</i> , 1981, 75, 1876-1887.	3.0	48
46	Fluorescence-dip infrared spectroscopy of the tropolone-H ₂ O complex. <i>Journal of Chemical Physics</i> , 1996, 105, 2605-2617.	3.0	47
47	An interatomic potential for mercury dimer. <i>Journal of Chemical Physics</i> , 2001, 114, 5545-5551.	3.0	47
48	Low-lying isomers and finite temperature behavior of (H ₂ O) ₆ . <i>Journal of Chemical Physics</i> , 2006, 125, 174301.	3.0	43
49	Comparison of models with distributed polarizable sites for describing water clusters. <i>Molecular Physics</i> , 2007, 105, 2681-2696.	1.7	42
50	Infrared predissociation spectroscopy of I ⁺ ⋯(CH ₃ OH) _n , n=1,2: Cooperativity in asymmetric solvation. <i>Journal of Chemical Physics</i> , 2002, 116, 4853.	3.0	41
51	Dominant structural motifs of NO ⁺ ⋯(H ₂ O) _n complexes: Infrared spectroscopic and ab initio studies. <i>Journal of Chemical Physics</i> , 2003, 118, 4945-4953.	3.0	41
52	Benchmark Calculations of the Energies for Binding Excess Electrons to Water Clusters. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 893-900.	5.3	39
53	Vibrational Spectroscopy of the Water-Nitrate Complex in the O-H Stretching Region. <i>Journal of Physical Chemistry A</i> , 2014, 118, 8188-8197.	2.5	39
54	Bonding in the Mg ₄ cluster. An example of chemical bonding originating from electron correlation effects. <i>Journal of Chemical Physics</i> , 1981, 75, 1044-1046.	3.0	37

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55	Molecular-level origin of the carboxylate head group response to divalent metal ion complexation at the air-water interface. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 14874-14880.	7.1	37
56	Establishing the Ground State of the Disjoint Diradical Tetramethyleneethane with Quantum Monte Carlo. Journal of the American Chemical Society, 2013, 135, 13862-13869.	13.7	34
57	A Self-Consistent Polarization Potential Model for Describing Excess Electrons Interacting with Water Clusters. Journal of Physical Chemistry B, 2013, 117, 4365-4370.	2.6	34
58	Theoretical approaches for treating non-valence correlation-bound anions. Journal of Chemical Physics, 2017, 147, 214114.	3.0	34
59	Computational Insight Concerning Catalytic Decision Points of the Transition Metal Catalyzed [2 + 2 + 1] Cyclocarbonylation Reaction of Allenes. Organometallics, 2006, 25, 5204-5206.	2.3	32
60	Exploring the correlation between network structure and electron binding energy in the (H ₂ O) ₇ ⁺ cluster through isomer-photoselected vibrational predissociation spectroscopy and <i>ab initio</i> calculations: Addressing complexity beyond types I-III. Journal of Chemical Physics, 2008, 128, 104314.	3.0	32
61	Isolating the Spectral Signatures of Individual Sites in Water Networks Using Vibrational Double-Resonance Spectroscopy of Cluster Isotopomers. Journal of Physical Chemistry Letters, 2010, 1, 2396-2401.	4.6	31
62	Mode-selective photoisomerization in 5-hydroxytropolone. II. Theory. Journal of Chemical Physics, 1995, 102, 5260-5270.	3.0	29
63	Correlation Consistent Gaussian Basis Sets for H, B, Ne with Dirac-Fock AREP Pseudopotentials: Applications in Quantum Monte Carlo Calculations. Journal of Chemical Theory and Computation, 2013, 9, 2170-2178.	5.3	27
64	Tag-Free and Isotopomer-Selective Vibrational Spectroscopy of the Cryogenically Cooled H ₉ O ₄ ⁺ Cation with Two-Color, IR-IR Double-Resonance Photoexcitation: Isolating the Spectral Signature of a Single OH Group in the Hydronium Ion Core. Journal of Physical Chemistry A, 2018, 122, 9275-9284.	2.5	27
65	Downsizing the Hydrated Electron's Lair. Science, 2010, 329, 42-43.	12.6	26
66	Quantum Monte Carlo calculation of the binding energy of the beryllium dimer. Journal of Chemical Physics, 2015, 143, 084116.	3.0	26
67	Characterization of the primary hydration shell of the hydroxide ion with H ₂ tagging vibrational spectroscopy of the OH ⁺ ... (H ₂ O) _n =2,3 and OD ⁺ ... (D ₂ O) _n =2,3 clusters. Journal of Chemical Physics, 2016, 145, 134304.	3.0	26
68	Theoretical studies of positron complexes with atomic anions. Journal of Chemical Physics, 1980, 72, 493-503.	3.0	25
69	Nonvalence Correlation-Bound Anion States of Spherical Fullerenes. Nano Letters, 2014, 14, 4602-4606.	9.1	25
70	Isolating the Charge-Transfer Component of the Anionic H Bond Via Spin Suppression of the Intracluster Proton Transfer Reaction in the NO-H ₂ O Entrance Channel Complex. Journal of Physical Chemistry A, 2002, 106, 10010-10014.	2.5	24
71	Evaluation of Theoretical Approaches for Describing the Interaction of Water with Linear Acenes. Journal of Physical Chemistry A, 2011, 115, 5955-5964.	2.5	24
72	Accurate Predictions of Electron Binding Energies of Dipole-Bound Anions via Quantum Monte Carlo Methods. Journal of Physical Chemistry Letters, 2018, 9, 6185-6190.	4.6	24

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109	Frontiers of stochastic electronic structure calculations. Journal of Chemical Physics, 2021, 154, 170401.	3.0	5
110	Near-Threshold Electron-Impact Excitation of the Low-Lying Rydberg States of Ethylene. Journal of Physical Chemistry A, 1999, 103, 5667-5670.	2.5	4
111	Exploration of Brueckner orbital trial wave functions in diffusion Monte Carlo calculations. Chemical Physics Letters, 2016, 644, 117-120.	2.6	4
112	Prediction of a Nonvalence Temporary Anion Shape Resonance for a Model (H ₂ O) ₄ System. Journal of Physical Chemistry A, 2019, 123, 2719-2726.	2.5	4
113	The role of high-order electron correlation effects in a model system for non-valence correlation-bound anions. Journal of Chemical Physics, 2020, 153, 224118.	3.0	4
114	Vibrational Signatures of HNO ₃ Acidity When Complexed with Microhydrated Alkali Metal Ions, M ⁺ ·(HNO ₃)(H ₂ O) _{n=5} (M = Li, K, Na, Rb, Cs), at 20 K. Journal of Physical Chemistry A, 2022, 126, 1640-1647.	2.5	4
115	Electron Transmission Study of the Splitting of the $\tilde{\nu}^*$ MO's of Angle-Strained Cyclic Acetylenes: Implications for the Electrophilicity of Alkynes. Bulletin Des Sociétés Chimiques Belges, 1982, 91, 363-363.	0.0	3
116	Diffusion Monte Carlo Study of the Parallel Displaced Form of the Benzene Dimer. ACS Symposium Series, 2016, , 107-117.	0.5	3
117	Theoretical Characterization of the Minimum-Energy Structure of (SF ₆) ₂ . Journal of Physical Chemistry B, 2016, 120, 1788-1792.	2.6	3
118	Prediction of a Non-Valence Temporary Anion State of (NaCl) ₂ . Journal of Physical Chemistry B, 2019, 123, 9198-9205.	2.6	3
119	Role of Overlap between the Discrete State and Pseudocontinuum States in Stabilization Calculations of Metastable States. Journal of Physical Chemistry A, 2021, 125, 4401-4408.	2.5	3
120	The binding of atomic hydrogen on graphene from density functional theory and diffusion Monte Carlo calculations. Journal of Chemical Physics, 2022, 156, 144702.	3.0	3
121	Determination of conformational preferences in biomolecule mimics with localized orbital coupled cluster methods. , 2012, , .		2
122	Implementation of analytical gradients and of a mixed real and momentum space DVR method for excess electron systems described by a self-consistent polarization model. Journal of Chemical Physics, 2017, 147, 161717.	3.0	2
123	Two-Dimensional Adiabatic Model for Calculating Progressions Resulting from Stretch-Rock Coupling in Vibrational Spectra of Anion-Water Complexes. Journal of Physical Chemistry Letters, 2021, 12, 6326-6329.	4.6	2
124	Real-Time Modulation of Hydrogen Evolution Activity of Graphene Electrodes Using Mechanical Strain. ACS Applied Materials & Interfaces, 2022, 14, 10691-10700.	8.0	2
125	Water Network Shape-Dependence of Local Interactions with the Microhydrated $\tilde{\nu}^*$ NO ₂ ⁺ and $\tilde{\nu}^*$ CO ₂ ⁺ Anionic Head Groups by Cold Ion Vibrational Spectroscopy. Journal of Physical Chemistry A, 2022, 126, 2471-2479.	2.5	2
126	An Effective In-Situ O ₂ High Density Plasma Clean. Materials Research Society Symposia Proceedings, 1993, 315, 273.	0.1	1

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127	Recent developments in electron-molecule scattering. International Journal of Quantum Chemistry, 1981, 20, 331-340.	2.0	1
128	Proton-coupled electron transfer in [pyridine \cdot (H ₂ O)] ⁿ⁺ , n= 3, 4, clusters. Chemical Physics Letters, 2016, 661, 196-199.	2.6	1
129	Going large(r): general discussion. Faraday Discussions, 2019, 217, 476-513.	3.2	1
130	Controlling internal degrees: general discussion. Faraday Discussions, 2019, 217, 138-171.	3.2	1
131	Pushing resolution in frequency and time: general discussion. Faraday Discussions, 2019, 217, 290-321.	3.2	1
132	Progress toward a one-electron model for the non-valence correlation-bound anions of polycyclic aromatic hydrocarbons. Electronic Structure, 2022, 4, 014010.	2.8	1
133	Exotic systems: general discussion. Faraday Discussions, 2019, 217, 601-622.	3.2	0
134	Analysis of the Contributions to the Kinetic and Potential Energies of an H Atom in the Presence of a Point Charge: The Molecular Virial Theorem Revisited. Journal of Physical Chemistry A, 2020, 124, 4534-4538.	2.5	0