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List of Publications by Year
in descending order

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Version: 2024-02-01

49 papers	15,721 citations	218381 26 h-index	223531 46 g-index
50 all docs	50 docs citations	50 times ranked	9559 citing authors

#	Article	IF	Citations
1	Theoretical kinetic studies of Venus chemistry. Formation and destruction of SCl, SCl2, and HSCl. Icarus, 2021, 354, 114051.	1.1	4
2	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. Journal of Physical Chemistry C, 2021, 125, 4342-4342.	1.5	0
3	Quantum Chemical Cluster Studies of Cationâ€“Ice Reactions for Astrochemical Applications: Seeking Experimental Confirmation. Accounts of Chemical Research, 2021, 54, 490-497.	7.6	11
4	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. Journal of Physical Chemistry A, 2021, 125, 1680-1680.	1.1	0
5	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. Journal of Physical Chemistry B, 2021, 125, 1973-1973.	1.2	0
6	The Formation of Glycolonitrile (HOCH₂CN) from Reactions of C⁺ with HCN and HNC on Icy Grain Mantles. Astrophysical Journal, 2021, 906, 20.	1.6	9
7	Formation of methyl ketenimine (CH3CHÂ=ÂCÂ=ÂNH) and ethylcyanide (CH3CH2Câ‰¡N) isomers through successive hydrogenations of acrylonitrile (CH2Â=ÂCHÂâˆ’ÂCâ‰¡N) under interstellar conditions: The role of CH3CÂ°HÂâˆ’ÂCâ‰¡N radical in the activation of the cyano group chemistry. Monthly Notices of the Royal Astronomical Society, 2019, 485, 5210-5220.	1.6	10
8	High level ab initio calculations on ClF n âˆ’ (n = 1â€“6): Recoupled pair bonding involving a closed-shell central ion. Computational and Theoretical Chemistry, 2017, 1116, 73-85.	1.1	4
9	Thom H. Dunning, Jr.: Contributions to chemical theory and computing. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	26
10	Quantum chemical protocols for modeling reactions and spectra in astrophysical ice analogs: the challenging case of the C⁺ + H₂O reaction in icy grain mantles. Physical Chemistry Chemical Physics, 2015, 17, 28705-28718.	1.3	8
11	Bonding in PF2Cl, PF3Cl, and PF4Cl: insight into isomerism and apicophilicity from ab initio calculations and the recoupled pair bonding model. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	8
12	Bonding in Sulfurâ€“Oxygen Compoundsâ€”HSO/SOH and SOO/OSO: An Example of Recoupled Pair Ï€ Bonding. Journal of Chemical Theory and Computation, 2013, 9, 4444-4452.	2.3	24
13	The First Row Anomaly and Recoupled Pair Bonding in the Halides of the Late p-Block Elements. Accounts of Chemical Research, 2013, 46, 359-368.	7.6	47
14	High Level ab Initio Calculations for ClF_n⁺ (n = 1â€“6) Ions: Refining the Recoupled Pair Bonding Model. Journal of Physical Chemistry A, 2013, 117, 4251-4266.	1.1	10
15	Insights into the Unusual Barrierless Reaction between Two Closed Shell Molecules, (CH₃)₂S + F₂, and Its H₂S + F₂ Analogue: Role of Recoupled Pair Bonding. Journal of Physical Chemistry A, 2012, 116, 5247-5255.	1.1	15
16	A Theoretical Investigation of the Plausibility of Reactions between Ammonia and Carbonyl Species (Formaldehyde, Acetaldehyde, and Acetone) in Interstellar Ice Analogs at Ultracold Temperatures. Journal of Physical Chemistry A, 2011, 115, 5166-5183.	1.1	30
17	ION-ICE ASTROCHEMISTRY: BARRIERLESS LOW-ENERGY DEPOSITION PATHWAYS TO HCOOH, CH₃OH, AND CO₂ON ICY GRAIN MANTLES FROM PRECURSOR CATIONS. Astrophysical Journal, 2011, 728, 44.	1.6	23
18	Gaussian basis sets for use in correlated molecular calculations. VII. Valence, core-valence, and scalar relativistic basis sets for Li, Be, Na, and Mg. Theoretical Chemistry Accounts, 2011, 128, 69-82.	0.5	536

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19	Hypervalency and recoupled pair bonding in the p-block elements. Computational and Theoretical Chemistry, 2011, 963, 7-12.	1.1	23
20	Recoupled Pair Bonding in PF_n(n= 1â^'5)^{â€}. Journal of Physical Chemistry A, 2010, 114, 8845-8851.	1.1	41
21	Modeling chemical growth processes in Titan's atmosphere 2. Theoretical study of reactions between C2H and ethene, propene, 1-butene, 2-butene, isobutene, trimethylethene, and tetramethylethene. Icarus, 2009, 202, 642-655.	1.1	32
22	Bonding in ClF_n (n = 1â^'7) Molecules: Further Insight into the Electronic Structure of Hypervalent Molecules and Recoupled Pair Bonds. Journal of Physical Chemistry A, 2009, 113, 12645-12654.	1.1	42
23	A comparison between polar covalent bonding and hypervalent recoupled pair bonding in diatomic chalcogen halide species {O,S,Se} Ã— {F,Cl,Br}. Molecular Physics, 2009, 107, 991-998.	0.8	42
24	Theory of Hypervalency: Recoupled Pair Bonding in SF_n (n = 1â^'6). Journal of Physical Chemistry A, 2009, 113, 7915-7926.	1.1	81
25	IS HO⁺₂A DETECTABLE INTERSTELLAR MOLECULE?. Astrophysical Journal, 2009, 697, 601-609.	1.6	35
26	Electron Affinity of NO. Journal of Physical Chemistry A, 2007, 111, 11185-11188.	1.1	26
27	Quantum Chemical Evaluation of the Astrochemical Significance of Reactions between S Atom and Acetylene or Ethylene. Journal of Physical Chemistry A, 2007, 111, 11249-11253.	1.1	13
28	Modeling chemical growth processes in Titanâ€™s atmosphere: 1. Theoretical rates for reactions between benzene and the ethynyl (C2H) and cyano (CN) radicals at low temperature and pressure. Chemical Physics, 2006, 331, 67-76.	0.9	43
29	Photoionization in ultraviolet processing of astrophysical ice analogs at cryogenic temperatures. Advances in Space Research, 2004, 33, 44-48.	1.2	14
30	Computational Confirmation of the Carrier for the "XCN" Interstellar Ice Band: OCN - Charge Transfer Complexes. Astrophysical Journal, 2004, 601, L63-L66.	1.6	22
31	Pathways to Glycine and Other Amino Acids in Ultraviolet-irradiated Astrophysical Ices Determined via Quantum Chemical Modeling. Astrophysical Journal, 2002, 571, L177-L180.	1.6	171
32	Ab initio quantum chemical studies of reactions in astrophysical ices. 4. Reactions in ices involving HCOOH, CH2NH, HCN, HNC, NH3, and H2O. International Journal of Quantum Chemistry, 2002, 88, 226-235.	1.0	35
33	Ab Initio Quantum Chemical Studies of Reactions in Astrophysical Ices 3. Reactions of HOCH2NH2Formed in H2CO/NH3/H2O Ices. Journal of Physical Chemistry A, 2001, 105, 9478-9481.	1.1	40
34	Benchmark calculations with correlated molecular wave functions. IX. The weakly bound complexes Arâ€“H2 and Arâ€“HCl. Journal of Chemical Physics, 1998, 109, 2233-2241.	1.2	46
35	The Rate of the Reaction between CN and C2H2at Interstellar Temperatures. Astrophysical Journal, 1997, 477, 204-208.	1.6	49
36	A correlated ab initio study of the Ãƒ2Î â†•XÌƒ2Î£+ transition in MgCCH. Chemical Physics Letters, 1997, 274, 299-305.	1.2	16

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37	The Rate of the Reaction between C2H and C2H2at Interstellar Temperatures. Astrophysical Journal, 1997, 489, 109-112.	1.6	35
38	Why HOC[TSUP]+[/TSUP] Is Detectable in Interstellar Clouds: The Rate of the Reaction between HOC[TSUP]+[/TSUP] and H[TINF]2[/TINF]. Astrophysical Journal, 1996, 463, L113-L115.	1.6	39
39	Ab initio investigation of the N2â€“HF complex: Accurate structure and energetics. Journal of Chemical Physics, 1996, 104, 5883-5891.	1.2	41
40	A correlated ab initio study of the XÌƒâ€‰2A1 and AÌƒâ€‰2E states of MgCH3. Journal of Chemical Physics, 1996, 104, 9495-9498.	1.2	9
41	An ab initio benchmark study of the H+COâ†'HCO reaction. Journal of Chemical Physics, 1996, 105, 9921-9926.	1.2	36
42	AB Initio Characterization of MgCCH, MgCCH +, and MgC 2 and Pathways to Their Formation in the Interstellar Medium. Astrophysical Journal, 1996, 456, 602.	1.6	50
43	On the Stability of Interstellar Carbon Clusters: The Rate of the Reaction between C 3 and O. Astrophysical Journal, 1996, 465, 795.	1.6	37
44	A correlated ab initio study of linear carbon-chain radicals CnH (n = 2â^'7). Chemical Physics Letters, 1995, 244, 45-52.	1.2	129
45	Gaussian basis sets for use in correlated molecular calculations. V. Coreâ€valence basis sets for boron through neon. Journal of Chemical Physics, 1995, 103, 4572-4585.	1.2	2,622
46	Ab Initio Modeling of (LiF)2 and (LiF)2(H2O). The Journal of Physical Chemistry, 1994, 98, 8831-8833.	2.9	6
47	Benchmark calculations with correlated molecular wave functions. V. The determination of accurate ab initio intermolecular potentials for He2, Ne2, and Ar2. Journal of Chemical Physics, 1994, 100, 2838-2850.	1.2	175
48	Gaussian basis sets for use in correlated molecular calculations. IV. Calculation of static electrical response properties. Journal of Chemical Physics, 1994, 100, 2975-2988.	1.2	2,382
49	Gaussian basis sets for use in correlated molecular calculations. III. The atoms aluminum through argon. Journal of Chemical Physics, 1993, 98, 1358-1371.	1.2	8,623