Jilai Li

List of Publications by Year in descending order

106 papers	2,218 citations	201385 27 h-index	276539 41 g-index
114 all docs	114 docs citations	114 times ranked	1622 citing authors

#	Article	IF	Citations
1	Electronic Effects on Room-Temperature, Gas-Phase Câ€“H Bond Activations by Cluster Oxides and Metal Carbides: The Methane Challenge. Journal of the American Chemical Society, 2017, 139, 17201-17212.	6.6	149
2	Electrostatic and Charge-Induced Methane Activation by a Concerted Double Câ€“H Bond Insertion. Journal of the American Chemical Society, 2017, 139, 1684-1689.	6.6	96
3	Unexpected Mechanistic Variants in the Thermal Gas-Phase Activation of Methane. Organometallics, 2017, 36, 8-17.	1.1	91
4	Electronic Origins of the Variable Efficiency of Room-Temperature Methane Activation by Homo- and Heteronuclear Cluster Oxide Cations [XYO₂]⁺ (X, Y = Al, Si, Mg): Competition between Proton-Coupled Electron Transfer and Hydrogen-Atom Transfer. Journal of the American Chemical Society, 2016, 138, 7973-7981.	6.6	90
5	Mechanistic Variants in Gas-Phase Metal-Oxide Mediated Activation of Methane at Ambient Conditions. Journal of the American Chemical Society, 2016, 138, 11368-11377.	6.6	85
6	Ta₂⁺-mediated ammonia synthesis from N₂and H₂at ambient temperature. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 11680-11687.	3.3	84
7	Bond Activation by Metalâ€“Carbene Complexes in the Gas Phase. Accounts of Chemical Research, 2016, 49, 494-502.	7.6	68
8	Control of Product Distribution and Mechanism by Ligation and Electric Field in the Thermal Activation of Methane. Angewandte Chemie - International Edition, 2017, 56, 10219-10223.	7.2	68
9	Complete cleavage of the Nâ‰¡N triple bond by Ta₂N⁺via degenerate ligand exchange at ambient temperature: A perfect catalytic cycle. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 21416-21420.	3.3	60
10	Hidden Hydride Transfer as a Decisive Mechanistic Step in the Reactions of the Unligated Gold Carbide [AuC]⁺ with Methane under Ambient Conditions. Angewandte Chemie - International Edition, 2016, 55, 13072-13075.	7.2	54
11	Large Density-Functional and Basis-Set Effects for the DMSO Reductase Catalyzed Oxo-Transfer Reaction. Journal of Chemical Theory and Computation, 2013, 9, 1799-1807.	2.3	42
12	Differences and Commonalities in the Gasâ€Phase Reactions of Closedâ€Shell Metal Dioxide Clusters [MO₂]⁺ (M=V, Nb, and Ta) with Methane. Chemistry - A European Journal, 2016, 22, 7225-7228.	1.7	39
13	Intrinsic Reactivity of Diatomic 3d Transition-Metal Carbides in the Thermal Activation of Methane: Striking Electronic Structure Effects. Journal of the American Chemical Society, 2019, 141, 599-610.	6.6	39
14	Ligandâ€Controlled CO₂ Activation Mediated by Cationic Titanium Hydride Complexes, [LTiH]⁺ (L=Cp₂, O). Chemistry - A European Journal, 2015, 21, 8483-8490.	1.7	38
15	On the Role of the Electronic Structure of the Heteronuclear Oxide Cluster [Ga₂Mg₂O₅]^{.+} in the Thermal Activation of Methane and Ethane: An Unusual Doping Effect. Angewandte Chemie - International Edition, 2015, 54, 5074-5078.	7.2	36
16	Spinâ€Selective Thermal Activation of Methane by Closedâ€Shell [TaO₃]⁺. Angewandte Chemie - International Edition, 2016, 55, 7257-7260.	7.2	36
17	Mechanism Insights of Ethane Câ€“H Bond Activations by Bare [FeIIIâ•O]+: Explicit Electronic Structure Analysis. Journal of Physical Chemistry A, 2012, 116, 1475-1485.	1.1	35
18	Large Equatorial Ligand Effects on Câ€“H Bond Activation by Nonheme Iron(IV)-oxo Complexes. Journal of Physical Chemistry B, 2014, 118, 1493-1500.	1.2	35

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19	Recent Advances in Iron-Catalyzed C-H Bond Activation Reactions. Current Inorganic Chemistry, 2012, 2, 64-85.	0.2	34
20	Efficient Roomâ€Temperature, Au⁺â€Mediated Coupling of a Carbene Ligand with Methane To Generate C₂H_x (x=4, 6). Angewandte Chemie - International Edition, 2016, 55, 441-444.	7.2	32
21	Mechanism of benzenehydroxylation by high-valent bare Fe^{iv}î€O²⁺: explicit electronic structure analysis. Physical Chemistry Chemical Physics, 2012, 14, 246-256.	1.3	30
22	Composition- and Size-Controlled Cyclic Self-Assembly by Solvent- and C₆₀-Responsive Self-Sorting. Journal of the American Chemical Society, 2013, 135, 15263-15268.	6.6	30
23	Benchmark Study on Methanol Câ€“H and Oâ€“H Bond Activation by Bare [Fe^{IV}O]²⁺. Journal of Physical Chemistry A, 2014, 118, 7146-7158.	1.1	30
24	Relay Stations for Electron Hole Migration in Peptides: Possibility for Formation of Three-Electron Bonds along Peptide Chains. Journal of Physical Chemistry B, 2008, 112, 14302-14311.	1.2	28
25	Aromatic Residues Regulating Electron Relay Ability of S-Containing Amino Acids by Formations of Sâ^Ï€ Multicenter Three-Electron Bonds in Proteins. Journal of Physical Chemistry C, 2012, 116, 19682-19688.	1.5	28
26	Activation of Methane and Carbon Dioxide Mediated by Transitionâ€Metal Doped Magnesium Oxide Clusters [MMgO]^{+/0/â^'} (M=Scâ€“Zn). Chemistry - A European Journal, 2015, 21, 7780-7789.	1.7	28
27	Electronic Enhancement Effect of Copper Modification of Base Pairs on the Conductivity of DNA. Journal of Physical Chemistry C, 2011, 115, 22547-22556.	1.5	27
28	Distinct Mechanistic Differences in the Hydrogenâ€Atom Transfer from Methane and Water by the Heteronuclear Oxide Cluster [Ga₂MgO₄]^{.+}. Angewandte Chemie - International Edition, 2015, 54, 12298-12302.	7.2	25
29	Sequential Gas-Phase Activation of Carbon Dioxide and Methane by [Re(CO)₂]⁺: The Sequence of Events Matters!. Journal of the American Chemical Society, 2017, 139, 6169-6176.	6.6	25
30	Artificial Cytochrome c Mimics: Graphene Oxideâ€“Fe(III) Complex-Coated Molecularly Imprinted Colloidosomes for Selective Photoreduction of Highly Toxic Pollutants. ACS Applied Materials & Interfaces, 2020, 12, 6615-6626.	4.0	25
31	Catalytic Cycle of Multicopper Oxidases Studied by Combined Quantum- and Molecular-Mechanical Free-Energy Perturbation Methods. Journal of Physical Chemistry B, 2015, 119, 8268-8284.	1.2	24
32	A quantum-mechanical study of the reaction mechanism of sulfite oxidase. Journal of Biological Inorganic Chemistry, 2014, 19, 1165-1179.	1.1	23
33	A Computational Comparison of Oxygen Atom Transfer Catalyzed by Dimethyl SulfÂoxide Reductase with Mo and W. European Journal of Inorganic Chemistry, 2015, 2015, 3580-3589.	1.0	23
34	Oriented external electric fields as mimics for probing the role of metal ions and ligands in the thermal gas-phase activation of methane. Dalton Transactions, 2018, 47, 15271-15277.	1.6	23
35	Hidden Hydride Transfer as a Decisive Mechanistic Step in the Reactions of the Unligated Gold Carbide [AuC]⁺ with Methane under Ambient Conditions. Angewandte Chemie, 2016, 128, 13266-13269.	1.6	22
36	A Reactionâ€Induced Localization of Spin Density Enables Thermal Câ^'H Bond Activation of Methane by Pristine FeC₄⁺. Chemistry - A European Journal, 2019, 25, 12940-12945.	1.7	22

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37	Efficient Roomâ€Temperature Activation of Methane by TaN⁺ under Câ^'N Coupling. Angewandte Chemie - International Edition, 2016, 55, 11678-11681.	7.2	21
38	The Unique Gasâ€Phase Chemistry of the [AuO]⁺/CH₄ Couple: Selective Oxygenâ€Atom Transfer to, Rather than Hydrogenâ€Atom Abstraction from, Methane. Angewandte Chemie - International Edition, 2016, 55, 10877-10880.	7.2	21
39	Striking Doping Effects on Thermal Methane Activation Mediated by the Heteronuclear Metal Oxides [XAlO₄]^{.+} (X=V, Nb, and Ta). Chemistry - A European Journal, 2017, 23, 788-792.	1.7	21
40	Thermal Dehydrogenation of Methane by [ReN]+. Angewandte Chemie - International Edition, 2016, 55, 14863-14866.	7.2	20
41	A Barrier-Free Atomic Radical-Molecule Reaction:â€‰ F + Propene. Journal of Chemical Theory and Computation, 2006, 2, 1551-1564.	2.3	19
42	On the Mechanisms of Hydrogenâ€Atom Transfer from Water to the Heteronuclear Oxide Cluster [Ga₂Mg₂O₅]^{.+}: Remarkable Electronic Structure Effects. Angewandte Chemie - International Edition, 2015, 54, 11861-11864.	7.2	19
43	SpinabhÃngige, thermische Aktivierung von Methan durch den geschlossenschaligen Cluster [TaO₃]⁺. Angewandte Chemie, 2016, 128, 7374-7377.	1.6	18
44	Thermal Activation of Methane by [HfO]^{.+} and [XHfO]⁺ (X=F, Cl, Br, I) and the Origin of a Remarkable Ligand Effect. Angewandte Chemie - International Edition, 2016, 55, 7685-7688.	7.2	18
45	Comparison of the Active-Site Design of Molybdenum Oxo-Transfer Enzymes by Quantum Mechanical Calculations. Inorganic Chemistry, 2014, 53, 11913-11924.	1.9	17
46	On the Origin of the Remarkably Variable Reactivities of [AlCeO_x]⁺ (x=2â€“4) towards Methane as a Function of Oxygen Content. Angewandte Chemie - International Edition, 2017, 56, 413-416.	7.2	17
47	Theoretical Elucidation of the Platinum-Mediated Arene Câ^'H Activation Reactions. Organometallics, 2007, 26, 2203-2210.	1.1	16
48	A Theoretical Study on Methane Câ€"H Bond Activation by Bare [FeO]^{+/0/â€“}. Journal of Physical Chemistry A, 2017, 121, 3501-3514.	1.1	16
49	Electronic promotion effect of double proton transfer on conduction of DNA through improvement of transverse electronic communication of base pairs. Journal of Chemical Physics, 2011, 135, 134315.	1.2	15
50	The Origin of the Efficient, Thermal Chemisorption of Methane by the Heteronuclear Metalâ€Oxide Cluster [Al₂TaO₅]⁺. Angewandte Chemie - International Edition, 2016, 55, 14867-14871.	7.2	15
51	Absorption and fluorescence emission spectroscopic characters of naphthoâ€homologated yyâ€DNA bases and effect of methanol solution and base pairing. Journal of Computational Chemistry, 2010, 31, 825-836.	1.5	14
52	Steuerung der Produktverteilung und der Mechanismen der thermischen Aktivierung von Methan durch Ligandeneffekte und elektrische Felder. Angewandte Chemie, 2017, 129, 10353-10357.	1.6	13
53	Thermal Oâ€"H Bond Activation of Water As Mediated by Heteronuclear [Al₂Mg₂O₅]^{â€¢+}: Evidence for Oxygen-Atom Scrambling. Journal of the American Chemical Society, 2018, 140, 9275-9281.	6.6	13
54	Carbonâ€Atom Extrusion from Halobenzenes and Its Coupling with a Methylene Ligand to Form Acetylene. Chemistry - A European Journal, 2015, 21, 9629-9631.	1.7	12

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55	Highly regioselective hydride transfer, oxidative dehydrogenation, and hydrogen-atom abstraction in the thermal gas-phase chemistry of [Zn(OH)]⁺/C₃H₈. Physical Chemistry Chemical Physics, 2014, 16, 26617-26623.	1.3	11
56	Direct Ab Initio Dynamics Study of Radical C₄H (X̃²Σ⁺) + CH₄ Reaction. Journal of Physical Chemistry A, 2011, 115, 3576-3582.	1.1	10
57	Direct ab initio dynamics study of the reaction of C₂(A³Π_u) with CH₄. International Journal of Quantum Chemistry, 2012, 112, 1078-1085.	1.0	10
58	Breaking and Making of Carbonâ€“Carbon Bonds by Lanthanides and Thirdâ€Row Transition Metals. Chemistry - A European Journal, 2016, 22, 3073-3076.	1.7	10
59	On the Origin of Roomâ€“temperature, Au⁺â€mediated Coupling of a Methylene Ligand with H₂. Implications for the Mechanism of Methane Dehydrogenation.. ChemistrySelect, 2016, 1, 444-447.	0.7	10
60	Zum Ursprung der effizienten thermischen Chemisorption von Methan durch den heteronuklearen Metalloxidcluster [Al₂TaO₅]⁺. Angewandte Chemie, 2016, 128, 15090-15094.	1.6	10
61	Counterâ€Intuitive Gasâ€Phase Reactivities of [V₂]⁺ and [V₂O]⁺ towards CO₂ Reduction: Insight from Electronic Structure Calculations. Angewandte Chemie - International Edition, 2020, 59, 12308-12314.	7.2	10
62	Deutlich unterschiedliche Mechanismen der Wasserstoffatomabstraktion aus Methan und Wasser durch den heteronuklearen Oxidcluster [Ga₂MgO₄]^{.+}. Angewandte Chemie, 2015, 127, 12472-12477.	1.6	9
63	Thermische Aktivierung von Methan durch [HfO]^{.+} und [XHfO]⁺ (X=F, Cl, Br,) Tj ETQq1 1 0.784314 rgBT /Ov	1.6	9
64	Thermische Dehydrierung von Methan durch [ReN]⁺. Angewandte Chemie, 2016, 128, 15085-15089.	1.6	9
65	On the Origin of Reactivity Enhancement/Suppression upon Sequential Ligation: [Re(CO)_x]⁺/CH₄ (x=0â€“3) Couples. Angewandte Chemie - International Edition, 2017, 56, 2951-2954.	7.2	9
66	Ursachen der unterschiedlichen ReaktivitÃt von [AlCeOx]+(x=2-4) gegenÃ¼ber Methan in AbhÃngigkeit vom Sauerstoffgehalt. Angewandte Chemie, 2017, 129, 424-428.	1.6	9
67	F/Cl+C2H2 reactions: Are the addition and hydrogen abstraction direct processes?. Chemical Physics, 2006, 331, 42-54.	0.9	8
68	Effiziente, thermische Aktivierung von Methan durch TaN⁺ unter Câ€Nâ€Kupplung. Angewandte Chemie, 2016, 128, 11851-11855.	1.6	8
69	A Theoretical Study on the Potential Energy Surface of the 1C3 + NO Reaction. Computational and Theoretical Chemistry, 2005, 730, 207-215.	1.5	7
70	Direct ab initio dynamics study of the reaction of C2(A3Îu) radical with C2H6. Chemical Physics Letters, 2011, 503, 210-214.	1.2	7
71	On the Crucial Role of Isolated Electronic States in the Thermal Reaction of ReC⁺ with Dihydrogen. Angewandte Chemie - International Edition, 2020, 59, 9370-9376.	7.2	7
72	A barrier-free atomâ€“molecule reaction: F + HONO. Chemical Physics, 2006, 324, 474-482.	0.9	6

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73	OH + HONO reaction: A theoretical study. Computational and Theoretical Chemistry, 2007, 847, 10-22.	1.5	6
74	Conformational transition pathway in the allosteric process of calciumâ€induced recoverin: Molecular dynamics simulations. Journal of Computational Chemistry, 2009, 30, 1135-1145.	1.5	6
75	Die Chemie von [AuO]⁺/CH₄ in der Gasphase: Selektive Sauerstoffatomâ€Âœbertragung auf, statt Wasserstoffatomâ€Abstraktion von Methan. Angewandte Chemie, 2016, 128, 11036-11039.	1.6	6
76	Reaction mechanisms of methanol oxidation by <scp>Fe^{IV}O</scp> biomimetic complex. International Journal of Quantum Chemistry, 2016, 116, 692-701.	1.0	6
77	Reassessment of the Mechanisms of Thermal Câ^'H Bond Activation of Methane by Cationic Magnesium Oxides: A Critical Evaluation of the Suitability of Different Density Functionals. ChemPhysChem, 2019, 20, 1812-1821.	1.0	5
78	Cl+HONO reaction: Are the hydrogen abstraction and addition direct/indirect processes?. Chemical Physics Letters, 2007, 441, 198-203.	1.2	4
79	Atomic radicalâ€"molecule reactions F +Â CH3Câ‰¡CH: mechanistic study. Theoretical Chemistry Accounts, 2007, 117, 417-429.	0.5	4
80	The Effects of Biological Environments on the Electronâ€Relay Functionality of Tryptophan Residues in Proteins. ChemPhysChem, 2012, 13, 183-192.	1.0	4
81	Mechanism Study of C₄H(X²â^'⁺)+H₂Reaction by DirectAb InitioMethods. Acta Chimica Sinica, 2013, 71, 743.	0.5	4
82	A barrier-free molecular radical-molecule reaction: $${^{3}C_{2} (a^{3}Pi) {+} O_{2} (X^{3}) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 382	0.5	3
83	Atomic radicalâ€"molecule reaction N (4S)+NO2 (2A1): Mechanistic study. Chemical Physics, 2009, 358, 80-84.	0.9	3
84	On the Crucial Role of Isolated Electronic States in the Thermal Reaction of ReC + with Dihydrogen. Angewandte Chemie, 2020, 132, 9456-9462.	1.6	3
85	CHAPTER 7. Computational Studies of Molybdenum and Tungsten Enzymes. 2-Oxoglutarate-Dependent Oxygenases, 2016, , 275-321.	0.8	3
86	â€œStrippingâ€•the Carbon Atom of Methyl Halide by a Cationic Holmium Complex: A Gasâ€Phase Study. Chemistry - A European Journal, 2015, 21, 14305-14308.	1.7	2
87	Frontispiece: Distinct Mechanistic Differences in the Hydrogen-Atom Transfer from Methane and Water by the Heteronuclear Oxide Cluster [Ga2MgO4].+. Angewandte Chemie - International Edition, 2015, 54, n/a-n/a.	7.2	2
88	Mechanistic Aspects of the Holmiumâ€Mediated, Reciprocal Hydrogen/Sulfur Exchange in the Gas Phase: C₆H₅CH₃+CH₂Sâ†'C₆H₅CHS+CH₄. Chemistry - A European Journal, 2016, 22, 4336-4339.	1.7	2
89	On the Origin of Reactivity Enhancement/Suppression upon Sequential Ligation: [Re(CO)_x]⁺/CH₄ (x=â€"3) Couples. Angewandte Chemie, 2017, 129, 2997-3000.	1.6	2
90	Revisiting the Intriguing Electronic Features of the BeOBeC Carbyne and Some Isomers: A Quantumâ€Chemical Assessment. Angewandte Chemie - International Edition, 2020, 59, 17261-17265.	7.2	2

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91	Experiment and Theory Clarify: Sc + Receives One Oxygen Atom from SO 2 to Form ScO + , which Proves to be a Catalyst for the Hidden Oxygenâ€Exchange with SO 2. ChemPhysChem, 2021, , .	1.0	2
92	Diatomic radicalâ€“molecule reactions CN + HONO: Mechanistic study. Computational and Theoretical Chemistry, 2008, 857, 20-26.	1.5	1
93	Theoretical elucidation of the rhodiumâ€catalyzed [4 + 2] annulation reactions. Journal of Computational Chemistry, 2008, 29, 686-693.	1.5	1
94	Mechanistic study on iron(II)â€mediated direct arylation of benzene with chlorobenzene. International Journal of Quantum Chemistry, 2019, 119, e25912.	1.0	1
95	Counterâ€Intuitive Gasâ€Phase Reactivities of [V₂]⁺ and [V₂O]⁺ towards CO₂ Reduction: Insight from Electronic Structure Calculations. Angewandte Chemie, 2020, 132, 12406-12412.	1.6	1
96	A Theoretical Study on Activation of Câ€”H and Câ€”Cl Bonds in CH₃X (X¼H, Cl) by Fe²⁺. Acta Chimica Sinica, 2012, 70, 1245.	0.5	1
97	A Theoretical Study of the Reaction of Fe⁺with CH₃X (X=Cl, Br, I). Acta Chimica Sinica, 2013, 71, 749.	0.5	1
98	Directab initiodynamics study of rate constants and kinetic isotope effects for C₂(A³Î_u)â€‰+â€‰CH₃OH reaction. Molecular Physics, 2012, 110, 2205-2217.	0.8	0
99	Direct ab initio study on the rate constants of radical C2(A3Îu)â€‰+â€‰C3H8 reaction. Journal of Molecular Modeling, 2013, 19, 1009-1018.	0.8	0
100	Theoretical Study of Methanol Câ€•H and Oâ€•H Bond Activation by PtRu Clusters. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2015, 31, 1077-1085.	2.2	0
101	Frontispiz: Deutlich unterschiedliche Mechanismen der Wasserstoffatomabstraktion aus Methan und Wasser durch den heteronuklearen Oxidcluster [Ga2MgO4].+. Angewandte Chemie, 2015, 127, n/a-n/a.	1.6	0
102	Frontispiece: Mechanistic Aspects of the Holmiumâ€Mediated, Reciprocal Hydrogen/Sulfur Exchange in the Gas Phase: C₆H₅CH₃+CH₂Sâ†'C₆H₅CHS+CH₄. Chemistry - A European Journal, 2016, 22, .	1.7	0
103	RÃ¼cktitelbild: Steuerung der Produktverteilung und der Mechanismen der thermischen Aktivierung von Methan durch Ligandeneffekte und elektrische Felder (Angew. Chem. 34/2017). Angewandte Chemie, 2017, 129, 10382-10382.	1.6	0
104	Frontispiece: Counterâ€Intuitive Gasâ€Phase Reactivities of [V₂]⁺ and [V₂O]⁺ towards CO₂ Reduction: Insight from Electronic Structure Calculations. Angewandte Chemie - International Edition, 2020, 59, .	7.2	0
105	Frontispiz: Counterâ€Intuitive Gasâ€Phase Reactivities of [V₂]⁺ and [V₂O]⁺ towards CO₂ Reduction: Insight from Electronic Structure Calculations. Angewandte Chemie, 2020, 132, .	1.6	0
106	Revisiting the Intriguing Electronic Features of the BeOBeC Carbyne and Some Isomers: A Quantumâ€Chemical Assessment. Angewandte Chemie, 2020, 132, 17414-17418.	1.6	0