Xin Xu

List of Publications by Citations

196 papers	9,522 citations	42 h-index	94 g-index
217 ext. papers	10,824 ext. citations	5.6 avg, IF	6.37 L-index

#	Paper	IF	Citations
196	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
195	From The Cover: The X3LYP extended density functional for accurate descriptions of nonbond interactions, spin states, and thermochemical properties. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 2673-7	11.5	782
194	ReaxFFSiO Reactive Force Field for Silicon and Silicon Oxide Systems. *Journal of Physical Chemistry A*, **2003**, 107, 3803-3811	2.8	682
193	Single-Atomic Cu with Multiple Oxygen Vacancies on Ceria for Electrocatalytic CO2 Reduction to CH4. *ACS Catalysis*, **2018**, 8, 7113-7119	13.1	323
192	Doubly hybrid density functional for accurate descriptions of nonbond interactions, thermochemistry, and thermochemical kinetics. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 4963-8	11.5	280
191	An extended hybrid density functional (X3LYP) with improved descriptions of nonbond interactions and thermodynamic properties of molecular systems. *Journal of Chemical Physics*, **2005**, 122, 14105	3.9	187
190	Chemical Enhancement Effects in SERS Spectra: A Quantum Chemical Study of Pyridine Interacting with Copper, Silver, Gold and Platinum Metals. *Journal of Physical Chemistry C*, **2008**, 112, 4195-4204	3.8	185
189	Doping strain induced bi-Ti pairs for efficient N activation and electrocatalytic fixation. *Nature Communications*, **2019**, 10, 2877	17.4	173
188	Bonding Properties of the Water Dimer:A Comparative Study of Density Functional Theories. *Journal of Physical Chemistry A*, **2004**, 108, 2305-2313	2.8	163
187	Boosting CO2 Electroreduction to CH4 via Tuning Neighboring Single-Copper Sites. *ACS Energy Letters*, **2020**, 5, 1044-1053	20.1	154
186	Extending the reliability and applicability of B3LYP. *Chemical Communications*, **2010**, 46, 3057-70	5.8	145
185	The extended Perdew-Burke-Ernzerhof functional with improved accuracy for thermodynamic and electronic properties of molecular systems. *Journal of Chemical Physics*, **2004**, 121, 4068-82	3.9	130
184	Accurate Energies and Structures for Large Water Clusters Using the X3LYP Hybrid Density Functional. *Journal of Physical Chemistry A*, **2004**, 108, 10518-10526	2.8	125
183	A fast doubly hybrid density functional method close to chemical accuracy using a local opposite spin ansatz. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 19896-900	11.5	124
182	Mechanisms of methane activation and transformation on molybdenum oxide based catalysts. *Journal of the American Chemical Society*, **2005**, 127, 3989-96	16.4	118
181	Performance of Several Density Functional Theory Methods on Describing Hydrogen-Bond Interactions. *Journal of Chemical Theory and Computation*, **2009**, 5, 86-96	6.4	117
180	Selective heterogeneous nucleation and growth of size-controlled metal nanoparticles on carbon nanotubes in solution. *Chemistry - A European Journal*, **2006**, 12, 2542-9	4.8	116

179	Benchmarking Density Functionals on Structural Parameters of Small-/Medium-Sized Organic Molecules. *Journal of Chemical Theory and Computation*, **2016**, 12, 459-65	6.4	110
178	OPBE: A promising density functional for the calculation of nuclear shielding constants. *Chemical Physics Letters*, **2006**, 421, 383-388	2.5	107
177	Doubly hybrid density functional for accurate description of thermochemistry, thermochemical kinetics and nonbonded interactions. *International Reviews in Physical Chemistry*, **2011**, 30, 115-160	7	106
176	Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0. *Journal of Chemical Physics*, **2012**, 136, 174103	3.9	86
175	The X1 method for accurate and efficient prediction of heats of formation. *Journal of Chemical Physics*, **2007**, 127, 214105	3.9	79
174	Self-assembly of normal alkanes on the Au (111) surfaces. *Chemistry - A European Journal*, **2004**, 10, 1415-22	4.8	79
173	One-Step Preparation of Large-Scale Self-Assembled Monolayers of Cyanuric Acid and Melamine Supramolecular Species on Au(111) Surfaces. *Journal of Physical Chemistry C*, **2008**, 112, 4209-4218	3.8	78
172	Chemisorption and Decomposition of Thiophene and Furan on the Si(100)-2 □1 Surface: A Quantum Chemical Study. *Journal of Physical Chemistry B*, **2001**, 105, 10069-10075	3.4	76
171	The gas phase reaction of singlet dioxygen with water: a water-catalyzed mechanism. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 3376-81	11.5	69
170	Geometric dependence of the B3LYP-predicted magnetic shieldings and chemical shifts. *Journal of Physical Chemistry A*, **2007**, 111, 9431-7	2.8	66
169	Systematic studies on the computation of nuclear magnetic resonance shielding constants and chemical shifts: the density functional models. *Journal of Computational Chemistry*, **2007**, 28, 2431-42	3.5	63
168	Reaching a Uniform Accuracy for Complex Molecular Systems: Long-Range-Corrected XYG3 Doubly Hybrid Density Functional. *Journal of Physical Chemistry Letters*, **2013**, 4, 1669-75	6.4	57
167	Mechanisms of initial propane activation on molybdenum oxides: a density functional theory study. *Journal of Physical Chemistry B*, **2005**, 109, 6416-21	3.4	57
166	Periodic trends in the bonding and vibrational coupling: Pyridine interacting with transition metals and noble metals studied by surface-enhanced Raman spectroscopy and density-functional theory. *Journal of Chemical Physics*, **2003**, 119, 1701-1709	3.9	57
165	Methane Activation by Transition-Metal Oxides, MOx (M = Cr, Mo, W; x = 1, 2, 3). *Journal of Physical Chemistry A*, **2002**, 106, 7171-7176	2.8	52
164	HHLA2 in intrahepatic cholangiocarcinoma: an immune checkpoint with prognostic significance and wider expression compared with PD-L1 **2019**, 7, 77		49
163	Theoretical Investigation on the Role of the Central Carbon Atom and Close Protein Environment on the Nitrogen Reduction in Mo Nitrogenase. *ACS Catalysis*, **2016**, 6, 1567-1577	13.1	49
162	Assessment of Handy□Cohen Optimized Exchange Density Functional (OPTX). *Journal of Physical Chemistry A*, **2004**, 108, 8495-8504	2.8	49

161	Construction of a parameter-free doubly hybrid density functional from adiabatic connection. *Journal of Chemical Physics*, **2014**, 140, 18A512	3.9	48
160	A hierarchical construction scheme for accurate potential energy surface generation: an application to the F+H2 reaction. *Journal of Chemical Physics*, **2008**, 129, 011103	3.9	48
159	Peroxone chemistry: formation of H2O3 and ring-(HO2)(HO3) from O3/H2O2. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 15308-12	11.5	47
158	XO: An extended ONIOM method for accurate and efficient geometry optimization of large molecules. *Chemical Physics Letters*, **2010**, 498, 203-208	2.5	46
157	Improving the B3LYP bond energies by using the X1 method. *Journal of Chemical Physics*, **2008**, 129, 164103	3.9	45
156	Fractional charge behavior and band gap predictions with the XYG3 type of doubly hybrid density functionals. *Journal of Physical Chemistry A*, **2014**, 118, 9201-11	2.8	43
155	Global Potential Energy Surface for the H+CH4<-H2+CH3 Reaction using Neural Networks. *Chinese Journal of Chemical Physics*, **2014**, 27, 373-379	0.9	43
154	Brønsted-NH(4)(+) mechanism versus nitrite mechanism: new insight into the selective catalytic reduction of NO by NH(3). *Physical Chemistry Chemical Physics*, **2011**, 13, 453-60	3.6	41
153	The XYG3 type of doubly hybrid density functionals. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 721-747	7.9	40
152	Chemisorption of acetonitrile, pyridine and pyrazine on the Si(100)-2×1 surface: theoretical predictions. *New Journal of Chemistry*, **2002**, 26, 160-164	3.6	40
151	Basis set dependence of the doubly hybrid XYG3 functional. *Journal of Chemical Physics*, **2010**, 133, 104105	3.9	39
150	Theoretical study of the vertical excited states of benzene, pyrimidine, and pyrazine by the symmetry adapted cluster--configuration interaction method. *Journal of Computational Chemistry*, **2007**, 28, 1658-67	3.5	38
149	XYG3s: Speedup of the XYG3 fifth-rung density functional with scaling-all-correlation method. *Journal of Chemical Physics*, **2010**, 132, 194105	3.9	37
148	Trends in R-X Bond Dissociation Energies (R = Me, Et, i-Pr, t-Bu, X = H, Me, Cl, OH). *Journal of Chemical Theory and Computation*, **2010**, 6, 1462-9	6.4	37
147	Hydrothermal Synthesis of New Pure Beryllophosphate Molecular Sieve Phases from Concentrated Amines. *Chemistry of Materials*, **2001**, 13, 2042-2048	9.6	36
146	Geometry optimization of Cn (n=2–30) with genetic algorithm. *Chemical Physics Letters*, **2002**, 364, 213-219	2.5	35
145	Bonding of NO2 to the Au Atom and Au(111) Surface: A Quantum Chemical Study. *Journal of Physical Chemistry A*, **1999**, 103, 10969-10974	2.8	34
144	Formation of Acrylates from Ethylene and CO2on Ni Complexes: A Mechanistic Viewpoint from a Hybrid DFT Approach. *Organometallics*, **2014**, 33, 6369-6380	3.8	33

143	Mechanisms for Selective Catalytic Oxidation of Ammonia over Vanadium Oxides. *Journal of Physical Chemistry C*, **2011**, 115, 21218-21229	3.8	33
142	Development of New Density Functional Approximations. *Annual Review of Physical Chemistry*, **2017**, 68, 155-182	15.7	32
141	Understanding the anion-π interactions with tetraoxacalix[2]arene[2]triazine. *Physical Chemistry Chemical Physics*, **2016**, 18, 6913-24	3.6	32
140	Nonfitting protein-ligand interaction scoring function based on first-principles theoretical chemistry methods: development and application on kinase inhibitors. *Journal of Computational Chemistry*, **2013**, 34, 1636-46	3.5	32
139	TiO2 sol-gel derived amperometric biosensor for H2O2 on the electropolymerized phenazine methosulfate modified electrode. *Analytical and Bioanalytical Chemistry*, **2002**, 374, 1261-6	4.4	32
138	N2O Decomposition on MgO and Li/MgO Catalysts: A Quantum Chemical Study. *Journal of Physical Chemistry B*, **1999**, 103, 3373-3379	3.4	32
137	Albumin to gamma-glutamyltransferase ratio as a prognostic indicator in intrahepatic cholangiocarcinoma after curative resection. *Oncotarget*, **2017**, 8, 13293-13303	3.3	30
136	XO: an extended ONIOM method for accurate and efficient modeling of large systems. *Journal of Computational Chemistry*, **2012**, 33, 2142-60	3.5	30
135	A comparison of geometric parameters from PBE-based doubly hybrid density functionals PBE0-DH, PBE0-2, and xDH-PBE0. *Journal of Chemical Physics*, **2013**, 139, 174106	3.9	30
134	Beyond Mean-Field Microkinetics: Toward Accurate and Efficient Theoretical Modeling in Heterogeneous Catalysis. *ACS Catalysis*, **2018**, 8, 5816-5826	13.1	29
133	XYG3 and XYGJ-OS performances for noncovalent binding energies relevant to biomolecular structures. *Physical Chemistry Chemical Physics*, **2012**, 14, 12554-70	3.6	29
132	Binding interaction analysis of the active site and its inhibitors for neuraminidase (N1 subtype) of human influenza virus by the integration of molecular docking, FMO calculation and 3D-QSAR CoMFA modeling. *Journal of Chemical Information and Modeling*, **2008**, 48, 1802-12	6.1	27
131	Understanding the reactivity of the tetrahedrally coordinated high-valence d0 transition metal oxides toward the C-H bond activation of alkanes: a cluster model study. *Journal of Physical Chemistry A*, **2008**, 112, 717-21	2.8	27
130	Accurate bond dissociation enthalpies by using doubly hybrid XYG3 functional. *Journal of Computational Chemistry*, **2011**, 32, 1824-38	3.5	25
129	Accurate prediction of heats of formation by a combined method of B3LYP and neural network correction. *Journal of Computational Chemistry*, **2009**, 30, 1424-44	3.5	25
128	Mechanism of methane oxidation by transition metal oxides: A cluster model study. *Catalysis Today*, **2006**, 117, 133-137	5.3	25
127	Theoretical studies on thermochemistry for conversion of 5-chloromethylfurfural into valuable chemicals. *Journal of Physical Chemistry A*, **2011**, 115, 13628-41	2.8	24
126	Janus Mesoporous Sensor Devices for Simultaneous Multivariable Gases Detection. *Matter*, **2019**, 1, 1274-1284	21.1	23

125	A new insight into the initial step in the Fischer-Tropsch synthesis: CO dissociation on Ru surfaces. *Physical Chemistry Chemical Physics*, **2012**, 14, 16686-94	3.6	23
124	The X1s method for accurate bond dissociation energies. *ChemPhysChem*, **2010**, 11, 2561-7	3.2	23
123	Self-assembly of alkanols on Au(111) surfaces. *Chemistry - A European Journal*, **2006**, 12, 4006-13	4.8	23
122	One Step Fabrication of Metal□Organic Coordination Monolayers on Au(111) Surfaces. *Journal of Physical Chemistry C*, **2007**, 111, 7570-7573	3.8	21
121	High charge flexibility of the surface dangling bonds on the Si(111)-7□7 surface and NH3 chemisorption: a DFT study. *Chemical Physics Letters*, **2002**, 355, 365-370	2.5	21
120	Electronic properties of metal nanorods probed by surface-enhanced Raman spectroscopy. *Chemical Communications*, **2000**, 1627-1628	5.8	21
119	Doubly hybrid density functionals that correctly describe both density and energy for atoms. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 2287-2292	11.5	20
118	Analytic derivatives for the XYG3 type of doubly hybrid density functionals: Theory, implementation, and assessment. *Journal of Computational Chemistry*, **2013**, 34, 1759-74	3.5	20
117	THEORETICAL STUDY OF GLYCINE CONFORMERS. *Journal of Theoretical and Computational Chemistry*, **2008**, 07, 889-909	1.8	20
116	ESI-MS and theoretical study on the coordination structures and reaction modes of the diperoxovanadate complexes containing histidine-like ligands. *International Journal of Mass Spectrometry*, **2008**, 269, 138-144	1.9	20
115	Double hybrid functionals and the □system bond length alternation challenge: rivaling accuracy of post-HF methods. *Journal of Chemical Theory and Computation*, **2015**, 11, 832-8	6.4	19
114	Gas-phase thermodynamics as a validation of computational catalysis on surfaces: a case study of Fischer-Tropsch synthesis. *ChemPhysChem*, **2012**, 13, 1486-94	3.2	19
113	DOX: A new computational protocol for accurate prediction of the protein-ligand binding structures. *Journal of Computational Chemistry*, **2016**, 37, 336-44	3.5	19
112	Toward the construction of parameter-free doubly hybrid density functionals. *International Journal of Quantum Chemistry*, **2015**, 115, 589-595	2.1	18
111	Selective Catalytic Dehydrogenative Oxidation of Bio-Polyols to Lactic Acid. *Angewandte Chemie - International Edition*, **2020**, 59, 13871-13878	16.4	18
110	Selective mono-N-methylation of nitroarenes with methanol catalyzed by atomically dispersed NHC-Ir solid assemblies. *Journal of Catalysis*, **2020**, 389, 337-344	7.3	18
109	A New-Generation Density Functional. *Springer Briefs in Molecular Science*, **2014**,	0.6	18
108	Pyrolysis of D-Glucose to Acrolein. *Chinese Journal of Chemical Physics*, **2011**, 24, 249-252	0.9	18

107	Density functional theory study of 1:1 glycine-water complexes in the gas phase and in solution. *Science China Chemistry*, **2010**, 53, 383-395	7.9	18
106	A time-dependent density functional theory investigation of the spectroscopic properties of the beta-subunit in C-phycocyanin. *Journal of Physical Chemistry B*, **2006**, 110, 18665-9	3.4	18
105	Prognostic Nomogram Based on Histological Characteristics of Fibrotic Tumor Stroma in Patients Who Underwent Curative Resection for Intrahepatic Cholangiocarcinoma. *Oncologist*, **2018**, 23, 1482-1493	5.7	18
104	Calculations of ionization energies and electron affinities for atoms and molecules: A comparative study with different methods. *Frontiers of Chemistry in China: Selected Publications From Chinese Universities*, **2011**, 6, 269-279		17
103	The X1 family of methods that combines B3LYP with neural network corrections for an accurate yet efficient prediction of thermochemistry. *International Journal of Quantum Chemistry*, **2015**, 115, 1021-1031	2.1	16
102	Accurate prediction of nuclear magnetic resonance shielding constants: towards the accuracy of CCSD(T) complete basis set limit. *Journal of Chemical Physics*, **2013**, 138, 124113	3.9	16
101	Hybrid molecular dynamics and first-principles study on the work function of a Pt(111) electrode immersed in aqueous solution at room temperature. *Physical Review B*, **2012**, 86,	3.3	16
100	Iridium-Catalyzed Selective Cross-Coupling of Ethylene Glycol and Methanol to Lactic Acid. *Angewandte Chemie - International Edition*, **2020**, 59, 10421-10425	16.4	15
99	Performance enhancement of dye-sensitized solar cells using an ester-functionalized imidazolium iodide as the solid state electrolyte. *ACS Applied Materials & Interfaces*, **2013**, 5, 3219-23	9.5	15
98	Mechanisms for NH3 Decomposition on the Si(111)-7 □7 Surface: A DFT Cluster Model Study. *Journal of Physical Chemistry C*, **2007**, 111, 16974-16981	3.8	15
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96	CASSCF study of bonding in NiCO and FeCO. *International Journal of Quantum Chemistry*, **1999**, 72, 221-231	2.1	15
95	Beyond energies: geometry predictions with the XYG3 type of doubly hybrid density functionals. *Chemical Communications*, **2016**, 52, 13840-13860	5.8	15
94	Exploring the Sodium Cation Location and Aluminum Distribution in ZSM-5: A Systematic Study by the Extended ONIOM (XO) Method. *Journal of Physical Chemistry C*, **2011**, 115, 14754-14761	3.8	14
93	Influence of reconstruction on the structure of self-assembled normal-alkane monolayers on Au(111) surfaces. *Physical Chemistry Chemical Physics*, **2002**, 4, 1486-1489	3.6	14
92	Highly Efficient and Selective N-Formylation of Amines with CO and H Catalyzed by Porous Organometallic Polymers. *Angewandte Chemie - International Edition*, **2021**, 60, 4125-4132	16.4	14
91	Integration approach at the second-order perturbation theory: applications to ionization potential and electron affinity calculations. *Journal of Chemical Theory and Computation*, **2015**, 11, 4677-88	6.4	13
90	Error accumulations in adhesive energies of dihydrogen molecular chains: performances of the XYG3 type of doubly hybrid density functionals. *Journal of Physical Chemistry A*, **2015**, 119, 1590-9	2.8	13

89	Isotopic Oxygen Exchange and EPR Studies of Superoxide Species on the SrF2/La2O3 Catalyst. *Catalysis Letters*, **2007**, 118, 238-243	2.8	13
88	Simultaneous Attenuation of Both Self-Interaction Error and Nondynamic Correlation Error in Density Functional Theory: A Spin-Pair Distinctive Adiabatic-Connection Approximation. *Journal of Physical Chemistry Letters*, **2019**, 10, 2617-2623	6.4	12
87	Understanding the Nonplanarity in Aromatic Metallabenzenes: A Control Mechanism. *Inorganic Chemistry*, **2018**, 57, 9205-9214	5.1	12
86	Bistability for CO Oxidation: An Understanding from Extended Phenomenological Kinetics Simulations. *ACS Catalysis*, **2019**, 9, 11116-11124	13.1	12
85	On the top rung of Jacob's ladder of density functional theory: Toward resolving the dilemma of SIE and NCE. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11,	7.9	12
84	The XPK package: A comparison between the extended phenomenological kinetic (XPK) method and the conventional kinetic Monte Carlo (KMC) method *Chinese Journal of Chemical Physics*, **2019**, 32, 143-150	0.9	11
83	Insights into Direct Methods for Predictions of Ionization Potential and Electron Affinity in Density Functional Theory. *Journal of Physical Chemistry Letters*, **2019**, 10, 2692-2699	6.4	11
82	Extended Koopmans' theorem at the second-order perturbation theory. *Journal of Computational Chemistry*, **2020**, 41, 1165-1174	3.5	11
81	Second-Order Perturbation Theory for Fractional Occupation Systems: Applications to Ionization Potential and Electron Affinity Calculations. *Journal of Chemical Theory and Computation*, **2016**, 12, 2285-97	6.4	11
80	H + H2 quantum dynamics using potential energy surfaces based on the XYG3 type of doubly hybrid density functionals: validation of the density functionals. *Journal of Chemical Physics*, **2015**, 142, 084107	3.9	10
79	A comparative study of the xDH-PBE0 and DSD-PBEPBE-D3BJ doubly hybrid density functionals. *Molecular Physics*, **2016**, 114, 1207-1217	1.7	10
78	Mechanisms for NH3 decomposition on Si(100)-(2 x 1) surface: a quantum chemical cluster model study. *Chemistry - A European Journal*, **2002**, 8, 5351-62	4.8	10
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76	Involvement of the Unoccupied Site Changes the Kinetic Trend Significantly: A Case Study on Formic Acid Decomposition. *ACS Catalysis*, **2020**, 10, 5153-5162	13.1	10
75	The harpooning mechanism as evidenced in the oxidation reaction of the Al atom. *Chemical Science*, **2018**, 9, 488-494	9.4	9
74	Ion strength and pH sensitive phase transition of N-isobutyryl-L-(D)-cysteine monolayers on Au(111) surfaces. *Langmuir*, **2010**, 26, 7343-8	4	9
73	Adsorbate lone-pair-electron stimulated charge transfer between surface dangling bonds: methanol chemisorption on Si(111)-7 . *Chemical Physics Letters*, **2004**, 388, 190-194	2.5	9
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65	How well can B3LYP heats of formation be improved by dispersion correction models?. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	7
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63	RRS-PBC: a molecular approach for periodic systems. *Science China Chemistry*, **2014**, 57, 1399-1404	7.9	7
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51	When does a functional correctly describe both the structure and the energy of the transition state?. *Journal of Molecular Modeling*, **2017**, 23, 65	2	5
50	High expression of Oct4 and Nanog predict poor prognosis in intrahepatic cholangiocarcinoma patients after curative resection. *Journal of Cancer*, **2019**, 10, 1313-1324	4.5	5
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48	Spectroscopic and DFT study on the interaction system of vanadium with L-proline in aqueous solution. *Journal of Physical Chemistry A*, **2010**, 114, 5211-6	2.8	5
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45	Enantioselective Rh-Catalyzed Hydroboration of Silyl Enol Ethers. *Journal of the American Chemical Society*, **2021**, 143, 10902-10909	16.4	5
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37	Selective Catalytic Dehydrogenative Oxidation of Bio-Polyols to Lactic Acid. *Angewandte Chemie*, **2020**, 132, 13975-13982	3.6	3
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