

Tanya K Todorova

List of Publications by Year in descending order

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48
papers

2,435
citations

185998

28
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197535

49
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52
all docs

52
docs citations

52
times ranked

3036
citing authors

#	ARTICLE	IF	CITATIONS
1	Mechanistic Understanding of CO ₂ Reduction Reaction (CO ₂ RR) Toward Multicarbon Products by Heterogeneous Copper-Based Catalysts. <i>ACS Catalysis</i> , 2020, 10, 1754-1768.	5.5	309
2	Electroreduction of CO ₂ to Formate with Low Overpotential using Cobalt Pyridine Thiolate Complexes. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 15726-15733.	7.2	38
3	Electroreduction of CO ₂ to Formate with Low Overpotential using Cobalt Pyridine Thiolate Complexes. <i>Angewandte Chemie</i> , 2020, 132, 15856-15863.	1.6	13
4	Synthetic and computational assessment of a chiral metal-organic framework catalyst for predictive asymmetric transformation. <i>Chemical Science</i> , 2020, 11, 8800-8808.	3.7	21
5	A bioinspired molybdenum-copper molecular catalyst for CO ₂ electroreduction. <i>Chemical Science</i> , 2020, 11, 5503-5510.	3.7	40
6	Metal-Metal Synergy in Well-Defined Surface Tantalum-Iridium Heterobimetallic Catalysts for H/D Exchange Reactions. <i>Journal of the American Chemical Society</i> , 2019, 141, 19321-19335.	6.6	33
7	Controlling Hydrogen Evolution during Photoreduction of CO ₂ to Formic Acid Using [Rh(R-bpy)(Cp*)Cl] ⁺ Catalysts: A Structure-Activity Study. <i>Inorganic Chemistry</i> , 2019, 58, 6893-6903.	1.9	31
8	A Bioinspired Nickel(bis-dithiolene) Complex as a Homogeneous Catalyst for Carbon Dioxide Electroreduction. <i>ACS Catalysis</i> , 2018, 8, 2030-2038.	5.5	86
9	Synthesis, Characterization, and DFT Analysis of Bis-Terpyridyl-Based Molecular Cobalt Complexes. <i>Inorganic Chemistry</i> , 2017, 56, 5930-5940.	1.9	52
10	New Cobalt-Bisterpyridyl Catalysts for Hydrogen Evolution Reaction. <i>ChemCatChem</i> , 2017, 9, 2099-2105.	1.8	36
11	A cobalt complex with a bioinspired molybdopterin-like ligand: a catalyst for hydrogen evolution. <i>Dalton Transactions</i> , 2016, 45, 14754-14763.	1.6	33
12	Octafluorodirhenate(III) Revisited: Solid-State Preparation, Characterization, and Multiconfigurational Quantum Chemical Calculations. <i>Inorganic Chemistry</i> , 2016, 55, 5417-5421.	1.9	6
13	Molecular Level Characterization of the Structure and Interactions in Peptide-Functionalized Metal-Organic Frameworks. <i>Chemistry - A European Journal</i> , 2016, 22, 16531-16538.	1.7	27
14	Molecular and Electronic Structure of Re ₂ Br ₄ (PMe ₃) ₄ . <i>Inorganic Chemistry</i> , 2016, 55, 7111-7116.	1.9	1
15	Connecting defects and amorphization in UiO-66 and MIL-140 metal-organic frameworks: a combined experimental and computational study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 2192-2201.	1.3	85
16	Bioinspired Tungsten Dithiolene Catalysts for Hydrogen Evolution: A Combined Electrochemical, Photochemical, and Computational Study. <i>Journal of Physical Chemistry B</i> , 2015, 119, 13524-13533.	1.2	37
17	Molecular and electronic structure of Tc ₂ (O ₂ CCH ₃) ₂ Cl ₄ studied by multiconfigurational quantum chemical methods. <i>Polyhedron</i> , 2014, 70, 144-147.	1.0	5
18	A Decade of Dinuclear Technetium Complexes with Multiple Metal-Metal Bonds. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 4484-4495.	1.0	5

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19	The Ligand-Based Quintuple Bond—Shortening Concept and Some of Its Limitations. <i>Chemistry - A European Journal</i> , 2013, 19, 9825-9832.	1.7	70
20	A multistep single-crystal-to-single-crystal bromodiacetylene dimerization. <i>Nature Chemistry</i> , 2013, 5, 327-334.	6.6	53
21	Volatilities of Actinide and Lanthanide N_2 -Dimethylaminodiboranate Chemical Vapor Deposition Precursors: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 23194-23200.	1.5	19
22	Biphasic water splitting by osmocene. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 11558-11563.	3.3	41
23	Multi-configurational quantum chemical studies of the $\text{Tc}_2\text{X}_8^{n-}$ ($\text{X} = \text{Cl}, \text{Br}; n = 2, 3$) anions. Crystallographic structure of octabromoditechnetate (3^-). <i>Dalton Transactions</i> , 2012, 41, 2869.	1.6	12
24	A Spectroscopic and Computational Study of a Photoinduced Cross-Dehydrogenative Coupling Reaction of a Stable Semiquinone Radical. <i>Chemistry - A European Journal</i> , 2012, 18, 13605-13608.	1.7	3
25	Synthesis and Properties of a Fifteen-Coordinate Complex: The Thorium Aminodiboranate $[\text{Th}(\text{H}_3\text{BNMe}_2)_3(\text{BH}_3)_4]$. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 3379-3381.	7.2	87
26	The $\text{cis-}\{\text{Ru}^{\text{II}}(\text{bpy})_2(\text{H}_2\text{O})_2\}^{2+}$ Water-Oxidation Catalyst Revisited. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 7745-7747.	7.2	107
27	DFT and CASPT2 Analysis of Polymetallic Uranium Nitride and Oxide Complexes: How Theory Can Help When X-Ray Analysis Is Inadequate. <i>Journal of the American Chemical Society</i> , 2010, 132, 12397-12403.	6.6	39
28	On the Analysis of the $\text{Cr}\sim\text{Cr}$ Multiple Bond in Several Classes of Dichromium Compounds. <i>Inorganic Chemistry</i> , 2010, 49, 5216-5222.	1.9	92
29	Structural, Spectroscopic, and Multiconfigurational Quantum Chemical Investigations of the Electron-Rich Metal-Metal Triple-Bonded $\text{Tc}_2\text{X}_4(\text{PMe}_3)_4$ ($\text{X} = \text{Cl}, \text{Br}$) Complexes. <i>Inorganic Chemistry</i> , 2010, 49, 6646-6654.	1.9	19
30	First emission studies of $\text{Tc}_2\text{X}_8^{n-}$ systems ($\text{X} = \text{Cl}, \text{Br}$). <i>Dalton Transactions</i> , 2010, 39, 11322.	1.6	12
31	Systematic truncation of the virtual space in multiconfigurational perturbation theory. <i>Journal of Chemical Physics</i> , 2009, 131, 034113.	1.2	50
32	Understanding, Controlling and Programming Cooperativity in Self-Assembled Polynuclear Complexes in Solution. <i>Chemistry - A European Journal</i> , 2009, 15, 12702-12718.	1.7	42
33	The chemiionization reactions $\text{Ce} + \text{O}$ and $\text{Ce} + \text{O}_2$: Assignment of the observed chemielectron bands. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2068-2079.	1.0	21
34	Vanadium Oxides Supported on a Thin Silica Film Grown on $\text{Mo}(112)$: Insights from Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2009, 113, 8336-8342.	1.5	17
35	The $\text{Ru}^{\text{II}}\text{Hbpp}$ Water Oxidation Catalyst. <i>Journal of the American Chemical Society</i> , 2009, 131, 15176-15187.	6.6	253
36	Formation of one-dimensional molybdenum oxide on $\text{Mo}(112)$. <i>Surface Science</i> , 2008, 602, 3338-3342.	0.8	23

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37	Theoretical Study of the Gas-Phase Chemiionization Reactions $\text{La} + \text{O}$ and $\text{La} + \text{O}_{2}$. Journal of Physical Chemistry A, 2008, 112, 7825-7830.	1.1	19
38	Nonuniform temperature dependence of the reactivity of disordered $\text{VOx}/\hat{\gamma}\text{-Al}_2\text{O}_3(001)$ surfaces: A density functional theory based Monte Carlo study. Journal of Chemical Physics, 2008, 129, 224710.	1.2	5
39	Oxygen adsorption on Mo(112) surface studied by ab initio genetic algorithm and experiment. Journal of Chemical Physics, 2007, 126, 234710.	1.2	37
40	Vanadium Oxides on Aluminum Oxide Supports. 3. Metastable $\hat{\gamma}\text{-Al}_2\text{O}_3(001)$ Compared to $\hat{\alpha}\text{-Al}_2\text{O}_3(0001)$. Journal of Physical Chemistry C, 2007, 111, 5141-5153.	1.5	27
41	On the geometrical and electronic structure of an ultra-thin crystalline silica film grown on Mo(112). Surface Science, 2007, 601, 4849-4861.	0.8	48
42	Interplay between theory and experiment in the quest for silica with reduced dimensionality grown on a Mo(112) surface. Chemical Physics Letters, 2006, 424, 115-119.	1.2	27
43	Formation of one-dimensional crystalline silica on a metal substrate. Surface Science, 2006, 600, L164-L168.	0.8	19
44	Low temperature adsorption of oxygen on reduced $\text{V}_2\text{O}_3(0001)$ surfaces. Surface Science, 2006, 600, 1497-1503.	0.8	55
45	Synthesis and Structure of Ultrathin Aluminosilicate Films. Angewandte Chemie - International Edition, 2006, 45, 7636-7639.	7.2	45
46	Atomic structure of a thin silica film on a Mo(112) substrate: A combined experimental and theoretical study. Physical Review B, 2006, 73, .	1.1	61
47	Atomic Structure of a Thin Silica Film on a Mo(112) Substrate: A Two-Dimensional Network of SiO_4 Tetrahedra. Physical Review Letters, 2005, 95, 076103.	2.9	201
48	Vanadium Oxides on Aluminum Oxide Supports. 1. Surface Termination and Reducibility of Vanadia Films on $\hat{\alpha}\text{-Al}_2\text{O}_3(0001)$. Journal of Physical Chemistry B, 2005, 109, 23523-23531.	1.2	42