Tanya K Todorova

List of Publications by Year in descending order

48 papers	2,435 citations	185998 28 h-index	197535 49 g-index
52 all docs	52 docs citations	52 times ranked	3036 citing authors

#	Article	IF	Citations
1	Mechanistic Understanding of CO₂ Reduction Reaction (CO2RR) Toward Multicarbon Products by Heterogeneous Copper-Based Catalysts. ACS Catalysis, 2020, 10, 1754-1768.	5.5	309
2	The Ruâ”Hbpp Water Oxidation Catalyst. Journal of the American Chemical Society, 2009, 131, 15176-15187.	6.6	253
3	Atomic Structure of a Thin Silica Film on a Mo(112) Substrate: A Two-Dimensional Network ofSiO4Tetrahedra. Physical Review Letters, 2005, 95, 076103.	2.9	201
4	The cisâ€[Ru^{II}(bpy)₂(H₂O)₂]²⁺ Waterâ€Oxidation Catalyst Revisited. Angewandte Chemie - International Edition, 2010, 49, 7745-7747.	7.2	107
5	On the Analysis of the Crâ”Cr Multiple Bond in Several Classes of Dichromium Compounds. Inorganic Chemistry, 2010, 49, 5216-5222.	1.9	92
6	Synthesis and Properties of a Fifteenâ€Coordinate Complex: The Thorium Aminodiboranate [Th(H₃BNMe₂BH₃)₄]. Angewandte Chemie - International Edition, 2010, 49, 3379-3381.	7.2	87
7	A Bioinspired Nickel(bis-dithiolene) Complex as a Homogeneous Catalyst for Carbon Dioxide Electroreduction. ACS Catalysis, 2018, 8, 2030-2038.	5.5	86
8	Connecting defects and amorphization in UiO-66 and MIL-140 metalâ€“organic frameworks: a combined experimental and computational study. Physical Chemistry Chemical Physics, 2016, 18, 2192-2201.	1.3	85
9	The Ligandâ€Based Quintuple Bondâ€Shortening Concept and Some of Its Limitations. Chemistry - A European Journal, 2013, 19, 9825-9832.	1.7	70
10	Atomic structure of a thin silica film on aMo(112)substrate: A combined experimental and theoretical study. Physical Review B, 2006, 73, .	1.1	61
11	Low temperature adsorption of oxygen on reduced V2O3(0001) surfaces. Surface Science, 2006, 600, 1497-1503.	0.8	55
12	A multistep single-crystal-to-single-crystal bromodiacetylene dimerization. Nature Chemistry, 2013, 5, 327-334.	6.6	53
13	Synthesis, Characterization, and DFT Analysis of Bis-Terpyridyl-Based Molecular Cobalt Complexes. Inorganic Chemistry, 2017, 56, 5930-5940.	1.9	52
14	Systematic truncation of the virtual space in multiconfigurational perturbation theory. Journal of Chemical Physics, 2009, 131, 034113.	1.2	50
15	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
16	Synthesis and Structure of Ultrathin Aluminosilicate Films. Angewandte Chemie - International Edition, 2006, 45, 7636-7639.	7.2	45
17	Vanadium Oxides on Aluminum Oxide Supports. 1. Surface Termination and Reducibility of Vanadia Films on Î±-Al2O3(0001). Journal of Physical Chemistry B, 2005, 109, 23523-23531.	1.2	42
18	Understanding, Controlling and Programming Cooperativity in Selfâ€Assembled Polynuclear Complexes in Solution. Chemistry - A European Journal, 2009, 15, 12702-12718.	1.7	42

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19	Biphasic water splitting by osmocene. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 11558-11563.	3.3	41
20	A bioinspired molybdenumâ€“copper molecular catalyst for CO₂ electroreduction. Chemical Science, 2020, 11, 5503-5510.	3.7	40
21	DFT and CASPT2 Analysis of Polymetallic Uranium Nitride and Oxide Complexes: How Theory Can Help When X-Ray Analysis Is Inadequate. Journal of the American Chemical Society, 2010, 132, 12397-12403.	6.6	39
22	Electroreduction of CO₂ to Formate with Low Overpotential using Cobalt Pyridine Thiolate Complexes. Angewandte Chemie - International Edition, 2020, 59, 15726-15733.	7.2	38
23	Oxygen adsorption on Mo(112) surface studied by ab initio genetic algorithm and experiment. Journal of Chemical Physics, 2007, 126, 234710.	1.2	37
24	Bioinspired Tungsten Dithiolene Catalysts for Hydrogen Evolution: A Combined Electrochemical, Photochemical, and Computational Study. Journal of Physical Chemistry B, 2015, 119, 13524-13533.	1.2	37
25	New Cobaltâ€Bisterpyridyl Catalysts for Hydrogen Evolution Reaction. ChemCatChem, 2017, 9, 2099-2105.	1.8	36
26	A cobalt complex with a bioinspired molybdopterin-like ligand: a catalyst for hydrogen evolution. Dalton Transactions, 2016, 45, 14754-14763.	1.6	33
27	Metalâ€“Metal Synergy in Well-Defined Surface Tantalumâ€“Iridium Heterobimetallic Catalysts for H/D Exchange Reactions. Journal of the American Chemical Society, 2019, 141, 19321-19335.	6.6	33
28	Controlling Hydrogen Evolution during Photoreduction of CO₂ to Formic Acid Using [Rh(R-bpy)(Cp*)Cl]⁺ Catalysts: A Structureâ€“Activity Study. Inorganic Chemistry, 2019, 58, 6893-6903.	1.9	31
29	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
30	Vanadium Oxides on Aluminum Oxide Supports. 3. Metastable Î²-Al2O3(001) Compared to Î±-Al2O3(0001). Journal of Physical Chemistry C, 2007, 111, 5141-5153.	1.5	27
31	Molecular Level Characterization of the Structure and Interactions in Peptideâ€Functionalized Metalâ€“Organic Frameworks. Chemistry - A European Journal, 2016, 22, 16531-16538.	1.7	27
32	Formation of one-dimensional molybdenum oxide on Mo(112). Surface Science, 2008, 602, 3338-3342.	0.8	23
33	The chemiionization reactions Ce + O and Ce + O₂: Assignment of the observed chemielectron bands. International Journal of Quantum Chemistry, 2009, 109, 2068-2079.	1.0	21
34	Synthetic and computational assessment of a chiral metalâ€“organic framework catalyst for predictive asymmetric transformation. Chemical Science, 2020, 11, 8800-8808.	3.7	21
35	Formation of one-dimensional crystalline silica on a metal substrate. Surface Science, 2006, 600, L164-L168.	0.8	19
36	Theoretical Study of the Gas-Phase Chemiionization Reactions La + O and La + O₂. Journal of Physical Chemistry A, 2008, 112, 7825-7830.	1.1	19

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37	Structural, Spectroscopic, and Multiconfigurational Quantum Chemical Investigations of the Electron-Rich Metalâ^'Metal Triple-Bonded Tc₂X₄(PMe₃)₄ (X = Cl, Br) Complexes. Inorganic Chemistry, 2010, 49, 6646-6654.	1.9	19
38	Volatilities of Actinide and Lanthanide N,N-Dimethylaminodiboranate Chemical Vapor Deposition Precursors: A DFT Study. Journal of Physical Chemistry C, 2012, 116, 23194-23200.	1.5	19
39	Vanadium Oxides Supported on a Thin Silica Film Grown on Mo(112): Insights from Density Functional Theory. Journal of Physical Chemistry C, 2009, 113, 8336-8342.	1.5	17
40	Electroreduction of CO 2 to Formate with Low Overpotential using Cobalt Pyridine Thiolate Complexes. Angewandte Chemie, 2020, 132, 15856-15863.	1.6	13
41	First emission studies of Tc2X82â^' systems (X = Cl, Br). Dalton Transactions, 2010, 39, 11322.	1.6	12
42	Multi-configurational quantum chemical studies of the Tc2X8nâ^' (X = Cl, Br; n = 2, 3) anions. Crystallographic structure of octabromoditechnetate(3â^'). Dalton Transactions, 2012, 41, 2869.	1.6	12
43	Octafluorodirhenate(III) Revisited: Solid-State Preparation, Characterization, and Multiconfigurational Quantum Chemical Calculations. Inorganic Chemistry, 2016, 55, 5417-5421.	1.9	6
44	Nonuniform temperature dependence of the reactivity of disordered VOx/Î²-Al2O3(001) surfaces: A density functional theory based Monte Carlo study. Journal of Chemical Physics, 2008, 129, 224710.	1.2	5
45	Molecular and electronic structure of Tc2(O2CCH3)2Cl4 studied by multiconfigurational quantum chemical methods. Polyhedron, 2014, 70, 144-147.	1.0	5
46	A Decade of Dinuclear Technetium Complexes with Multiple Metal-Metal Bonds. European Journal of Inorganic Chemistry, 2014, 2014, 4484-4495.	1.0	5
47	A Spectroscopic and Computational Study of a Photoinduced Crossâ€Dehydrogenative Coupling Reaction of a Stable Semiquinone Radical. Chemistry - A European Journal, 2012, 18, 13605-13608.	1.7	3
48	Molecular and Electronic Structure of Re2Br4(PMe3)4. Inorganic Chemistry, 2016, 55, 7111-7116.	1.9	1