Simone Raugei

List of Publications by Year
in descending order

116 papers	5,122 citations	57719 44 h-index	98753 67 g-index
119 all docs	119 docs citations	119 times ranked	4636 citing authors

#	Article	IF	Citations
1	Reduction of Substrates by Nitrogenases. Chemical Reviews, 2020, 120, 5082-5106.	23.0	234
2	Triggering dynamics of the high-pressure benzene amorphization. Nature Materials, 2007, 6, 39-43.	13.3	197
3	Moving Protons with Pendant Amines: Proton Mobility in a Nickel Catalyst for Oxidation of Hydrogen. Journal of the American Chemical Society, 2011, 133, 14301-14312.	6.6	151
4	Homogenous Electrocatalytic Oxygen Reduction Rates Correlate with Reaction Overpotential in Acidic Organic Solutions. ACS Central Science, 2016, 2, 850-856.	5.3	150
5	An ab initio study of water molecules in the bromide ion solvation shell. Journal of Chemical Physics, 2002, 116, 196.	1.2	141
6	High Catalytic Rates for Hydrogen Production Using Nickel Electrocatalysts with Seven-Membered Cyclic Diphosphine Ligands Containing One Pendant Amine. Journal of the American Chemical Society, 2013, 135, 6033-6046.	6.6	137
7	The radical mechanism of biological methane synthesis by methyl-coenzyme M reductase. Science, 2016, 352, 953-958.	6.0	129
8	Proton Delivery and Removal in [Ni(P^R₂N^{R^{â€²}}₂)₂]²⁺ Hydrogen Production and Oxidation Catalysts. Journal of the American Chemical Society, 2012, 134, 19409-19424.	6.6	122
9	Hydrogen oxidation catalysis by a nickel diphosphine complex with pendant tert-butyl amines. Chemical Communications, 2010, 46, 8618.	2.2	107
10	Distant protonated pyridine groups in water-soluble iron porphyrin electrocatalysts promote selective oxygen reduction to water. Chemical Communications, 2012, 48, 11100.	2.2	104
11	The Role of Pendant Amines in the Breaking and Forming of Molecular Hydrogen Catalyzed by Nickel Complexes. Chemistry - A European Journal, 2012, 18, 6493-6506.	1.7	102
12	Energy Transduction in Nitrogenase. Accounts of Chemical Research, 2018, 51, 2179-2186.	7.6	101
13	Critical computational analysis illuminates the reductive-elimination mechanism that activates nitrogenase for N ₂ reduction. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E10521-E10530.	3.3	100
14	Mechanism of Catalytic O₂ Reduction by Iron Tetraphenylporphyrin. Journal of the American Chemical Society, 2019, 141, 8315-8326.	6.6	99
15	Calculation of Redox Properties:â€‰ Understanding Short- and Long-Range Effects in Rubredoxin. Journal of Physical Chemistry B, 2007, 111, 3969-3976.	1.2	88
16	Polarization effects and charge transfer in the KcsA potassium channel. Biophysical Chemistry, 2006, 124, 292-301.	1.5	84
17	Comprehensive Thermodynamics of Nickel Hydride Bis(Diphosphine) Complexes: A Predictive Model through Computations. Organometallics, 2011, 30, 6108-6118.	1.1	76
18	Solute-Solvent Charge Transfer in Aqueous Solution. ChemPhysChem, 2005, 6, 1715-1718.	1.0	75

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19	Incorporating Peptides in the Outer-Coordination Sphere of Bioinspired Electrocatalysts for Hydrogen Production. Inorganic Chemistry, 2011, 50, 4073-4085.	1.9	73
20	Molecular dynamics study of the proposed proton transport pathways in [FeFe]-hydrogenase. Biochimica Et Biophysica Acta - Bioenergetics, 2014, 1837, 131-138.	0.5	71
21	Nuclear Quantum Effects and Hydrogen Bonding in Liquids. Journal of the American Chemical Society, 2003, 125, 8992-8993.	6.6	70
22	Hydrogen Production Using Nickel Electrocatalysts with Pendant Amines: Ligand Effects on Rates and Overpotentials. ACS Catalysis, 2013, 3, 2527-2535.	5.5	70
23	Structure and Function of Vanadium Haloperoxidasesâ€. Journal of Physical Chemistry B, 2006, 110, 3747-3758.	1.2	68
24	Computing Free Energy Landscapes: Application to Ni-based Electrocatalysts with Pendant Amines for H₂ Production and Oxidation. ACS Catalysis, 2014, 4, 229-242.	5.5	68
25	Pressure-Induced Frustration and Disorder inMg(OH)2andCa(OH)2. Physical Review Letters, 1999, 83, 2222-2225.	2.9	67
26	Experimental and Computational Mechanistic Studies Guiding the Rational Design of Molecular Electrocatalysts for Production and Oxidation of Hydrogen. Inorganic Chemistry, 2016, 55, 445-460.	1.9	67
27	Stabilization of Nickel Complexes with Ni0Â·Â·Â·Hâ€“N Bonding Interactions Using Sterically Demanding Cyclic Diphosphine Ligands. Organometallics, 2012, 31, 144-156.	1.1	66
28	Toward Molecular Catalysts by Computer. Accounts of Chemical Research, 2015, 48, 248-255.	7.6	65
29	Convergent Dynamics in the Protease Enzymatic Superfamily. Journal of the American Chemical Society, 2006, 128, 9766-9772.	6.6	61
30	Dynamics of Water Molecules in the Br-Solvation Shell:Â An ab Initio Molecular Dynamics Study. Journal of the American Chemical Society, 2001, 123, 9484-9485.	6.6	59
31	High-Resolution ENDOR Spectroscopy Combined with Quantum Chemical Calculations Reveals the Structure of Nitrogenase Janus Intermediate E₄(4H). Journal of the American Chemical Society, 2019, 141, 11984-11996.	6.6	58
32	On the Zwitterionic Nature of Gas-Phase Peptides and Protein Ions. PLoS Computational Biology, 2010, 6, e1000775.	1.5	56
33	Molecular Dynamics in Physiological Solutions: Force Fields, Alkali Metal Ions, and Ionic Strength. Journal of Chemical Theory and Computation, 2010, 6, 2167-2175.	2.3	56
34	Tuning Catalytic Bias of Hydrogen Gas Producing Hydrogenases. Journal of the American Chemical Society, 2020, 142, 1227-1235.	6.6	55
35	Ammonia Oxidation by Abstraction of Three Hydrogen Atoms from a Moâ€“NH₃ Complex. Journal of the American Chemical Society, 2017, 139, 2916-2919.	6.6	54
36	A new era for electron bifurcation. Current Opinion in Chemical Biology, 2018, 47, 32-38.	2.8	54

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37	Relative pKaValues from First-Principles Molecular Dynamics:Â The Case of Histidine Deprotonation. Journal of Physical Chemistry B, 2006, 110, 6365-6371.	1.2	52
38	Mechanism of Nitrogenase H₂ Formation by Metal-Hydride Protonation Probed by Mediated Electrocatalysis and H/D Isotope Effects. Journal of the American Chemical Society, 2017, 139, 13518-13524.	6.6	51
39	Formamide Hydrolysis Investigated by Multiple-Steering ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2004, 108, 369-375.	1.2	50
40	Achieving Reversible H₂/H⁺ Interconversion at Room Temperature with Enzyme-Inspired Molecular Complexes: A Mechanistic Study. ACS Catalysis, 2016, 6, 6037-6049.	5.5	49
41	Controlling Proton Delivery through Catalyst Structural Dynamics. Angewandte Chemie - International Edition, 2016, 55, 13509-13513.	7.2	48
42	Molecular Catalysts with Diphosphine Ligands Containing Pendant Amines. Chemical Reviews, 2022, 122, 12427-12474.	23.0	48
43	Iron Complexes for the Electrocatalytic Oxidation of Hydrogen: Tuning Primary and Secondary Coordination Spheres. ACS Catalysis, 2014, 4, 1246-1260.	5.5	47
44	CO₂ Reduction Catalyzed by Nitrogenase: Pathways to Formate, Carbon Monoxide, and Methane. Inorganic Chemistry, 2016, 55, 8321-8330.	1.9	47
45	Microsolvation effect on chemical reactivity: The case of the Clâ^'+CH3Br SN2 reaction. Journal of Chemical Physics, 2001, 114, 4089-4098.	1.2	46
46	Homogeneous Ni Catalysts for H2Oxidation and Production: An Assessment of Theoretical Methods, from Density Functional Theory to Post Hartreeâ^'Fock Correlated Wave-Function Theory. Journal of Physical Chemistry A, 2010, 114, 12716-12724.	1.1	44
47	Structural characterization of the P1+ intermediate state of the P-cluster of nitrogenase. Journal of Biological Chemistry, 2018, 293, 9629-9635.	1.6	44
48	Manganese-Based Molecular Electrocatalysts for Oxidation of Hydrogen. ACS Catalysis, 2015, 5, 6838-6847.	5.5	43
49	Control of electron transfer in nitrogenase. Current Opinion in Chemical Biology, 2018, 47, 54-59.	2.8	43
50	A Computational Model for Protein Ionization by Electrospray Based on Gas-Phase Basicity. Journal of the American Society for Mass Spectrometry, 2012, 23, 1903-1910.	1.2	42
51	Negative cooperativity in the nitrogenase Fe protein electron delivery cycle. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E5783-E5791.	3.3	42
52	Photoinduced Reductive Elimination of H₂ from the Nitrogenase Dihydride (Janus) State Involves a FeMo-cofactor-H₂ Intermediate. Inorganic Chemistry, 2017, 56, 2233-2240.	1.9	42
53	Selectivity-Determining Steps in O₂ Reduction Catalyzed by Iron(tetramesitylporphyrin). Journal of the American Chemical Society, 2020, 142, 4108-4113.	6.6	41
54	Comment on â€œNew Insights in the Electrocatalytic Proton Reduction and Hydrogen Oxidation by Bioinspired Catalysts: A DFT Investigationâ€• Journal of Physical Chemistry A, 2011, 115, 4861-4865.	1.1	40

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55	Increasing the rate of hydrogen oxidation without increasing the overpotential: a bio-inspired iron molecular electrocatalyst with an outer coordination sphere proton relay. Chemical Science, 2015, 6, 2737-2745.	3.7	40
56	The Role of a Dipeptide Outerâ€Coordination Sphere on H₂â€Production Catalysts: Influence on Catalytic Rates and Electron Transfer. Chemistry - A European Journal, 2013, 19, 1928-1941.	1.7	38
57	Fe Protein-Independent Substrate Reduction by Nitrogenase MoFe Protein Variants. Biochemistry, 2015, 54, 2456-2462.	1.2	38
58	Ab Initio-Based Kinetic Modeling for the Design of Molecular Catalysts: The Case of H₂ Production Electrocatalysts. ACS Catalysis, 2015, 5, 5436-5452.	5.5	38
59	Conformational Dynamics and Proton Relay Positioning in Nickel Catalysts for Hydrogen Production and Oxidation. Organometallics, 2013, 32, 7034-7042.	1.1	36
60	Controlling proton movement: electrocatalytic oxidation of hydrogen by a nickel(<scp>ii</scp>) complex containing proton relays in the second and outer coordination spheres. Dalton Transactions, 2014, 43, 2744-2754.	1.6	35
61	An ab initio molecular dynamics study of the SN2 reaction Clâ^'+CH3Brâ†'CH3Cl+Brâ^'. Journal of Chemical Physics, 1999, 111, 10887-10894.	1.2	34
62	Enzyme Design from the Bottom Up: An Active Nickel Electrocatalyst with a Structured Peptide Outer Coordination Sphere. Chemistry - A European Journal, 2014, 20, 1510-1514.	1.7	34
63	Incorporating Amino Acid Esters into Catalysts for Hydrogen Oxidation: Steric and Electronic Effects and the Role of Water as a Base. Organometallics, 2012, 31, 6719-6731.	1.1	33
64	Electron Redistribution within the Nitrogenase Active Site FeMo-Cofactor During Reductive Elimination of H₂ to Achieve Nâ‰¡N Triple-Bond Activation. Journal of the American Chemical Society, 2020, 142, 21679-21690.	6.6	32
65	Single-Amino Acid Modifications Reveal Additional Controls on the Proton Pathway of [FeFe]-Hydrogenase. Biochemistry, 2016, 55, 3165-3173.	1.2	29
66	Substrate Channel in Nitrogenase Revealed by a Molecular Dynamics Approach. Biochemistry, 2014, 53, 2278-2285.	1.2	28
67	Water-assisted proton delivery and removal in bio-inspired hydrogen production catalysts. Dalton Transactions, 2015, 44, 10969-10979.	1.6	28
68	Design and reactivity of pentapyridyl metal complexes for ammonia oxidation. Chemical Communications, 2019, 55, 5083-5086.	2.2	27
69	A Proficient Enzyme:Â Insights on the Mechanism of Orotidine Monophosphate Decarboxylase from Computer Simulations. Journal of the American Chemical Society, 2004, 126, 15730-15737.	6.6	26
70	Optimizing conditions for utilization of an H₂ oxidation catalyst with outer coordination sphere functionalities. Dalton Transactions, 2016, 45, 9786-9793.	1.6	26
71	Carâ€"Parrinello molecular dynamics on the SN2 reaction Clâ^'+CH3Br in water. Computational and Theoretical Chemistry, 2003, 630, 141-149.	1.5	24
72	Ab- initio molecular dynamics study of the SN2 reaction Cl- + ClCH2CN. Physical Chemistry Chemical Physics, 2001, 3, 2559-2566.	1.3	21

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73	Role of the Subunit Interactions in the Conformational Transitions in Adult Human Hemoglobin: An Explicit Solvent Molecular Dynamics Study. Journal of Physical Chemistry B, 2012, 116, 11004-11009.	1.2	21
74	Ab Initio Molecular Dynamics Investigation of the Formyl Cation in the Superacid SbF5/HF. Journal of Physical Chemistry B, 2001, 105, 8212-8219.	1.2	20
75	Intramolecular Electrostatic Effects on O₂, CO₂, and Acetate Binding to a Cationic Iron Porphyrin. Inorganic Chemistry, 2020, 59, 17402-17414.	1.9	20
76	On the Quantum Nature of an Excess Proton in Liquid Hydrogen Fluoride. ChemPhysChem, 2004, 5, 1569-1576.	1.0	19
77	Hydrocarbon Reactivity in the Superacid SbF5/HF:Â an ab Initio Molecular Dynamics Study. Journal of Physical Chemistry B, 2002, 106, 11596-11605.	1.2	18
78	Ab Initio Raman Spectra of Î²-Lactamase Inhibitor Intermediates Bound to E166A SHV Î²-Lactamase. Journal of Chemical Theory and Computation, 2009, 5, 2158-2172.	2.3	17
79	Synthesis and Reactivity of Tripodal Complexes Containing Pendant Bases. Inorganic Chemistry, 2014, 53, 9242-9253.	1.9	16
80	DFT modeling of biological systems. Physica Status Solidi (B): Basic Research, 2006, 243, 2500-2515.	0.7	15
81	Investigating the role of chain and linker length on the catalytic activity of an H₂ production catalyst containing a Î²-hairpin peptide. Journal of Coordination Chemistry, 2016, 69, 1730-1747.	0.8	15
82	Catalytic bias in oxidationâ€“reduction catalysis. Chemical Communications, 2021, 57, 713-720.	2.2	15
83	Anion control of tautomeric equilibria: Feâ€“H vs. Nâ€“H influenced by NHâ‹¯F hydrogen bonding. Chemical Science, 2019, 10, 1410-1418.	3.7	14
84	CarÃ¢â‚¬â€œParrinello molecular dynamics of the SN2 reaction ClÃ¢â‚¬â€œÃ¢â‚¬â€+Ã¢â‚¬â€Cl2CH2. Physical Chemistry Chemical Physics, 2001, 3, 4870-4873.	1.3	13
85	Molecular Simulation-Based Structural Prediction of Protein Complexes in Mass Spectrometry: The Human Insulin Dimer. PLoS Computational Biology, 2014, 10, e1003838.	1.5	13
86	Controlling Proton Delivery through Catalyst Structural Dynamics. Angewandte Chemie, 2016, 128, 13707-13711.	1.6	12
87	Nickelâ€“Sulfonate Mode of Substrate Binding for Forward and Reverse Reactions of Methyl-SCoM Reductase Suggest a Radical Mechanism Involving Long-Range Electron Transfer. Journal of the American Chemical Society, 2021, 143, 5481-5496.	6.6	12
88	Structure of the strongly associated liquid antimony pentafluoride: An ab initio molecular dynamics study. Journal of Chemical Physics, 2002, 116, 7087-7093.	1.2	11
89	Structure and Raman Spectrum of Clavulanic Acid in Aqueous Solution. Journal of Physical Chemistry B, 2007, 111, 2621-2630.	1.2	11
90	Chokepoints in Mechanical Coupling Associated with Allosteric Proteins: The Pyruvate Kinase Example. Biophysical Journal, 2019, 116, 1598-1608.	0.2	10

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91	Mechanical Stabilization Effect of Water on a Membrane-like System. Journal of the American Chemical Society, 2007, 129, 2636-2641.	6.6	9
92	Covalent Functionalization of Nickel Phosphide Nanocrystals with Aryl-Diazonium Salts. Chemistry of Materials, 2021, 33, 9652-9665.	3.2	9
93	Mechanical coupling in the nitrogenase complex. PLoS Computational Biology, 2021, 17, e1008719.	1.5	8
94	Orientational ordering in the mixed crystal Ar1â^'x(N2)x: A molecular dynamics study. Journal of Chemical Physics, 1997, 106, 8196-8203.	1.2	7
95	Structure and Bonding in Monomeric Iron(III) Complexes with Terminal Oxo and Hydroxo Ligands. Inorganic Chemistry, 2006, 45, 1732-1738.	1.9	7
96	Evaluation of the Role of Water in the H₂ Bond Formation by Ni(II)-Based Electrocatalysts. Journal of Chemical Theory and Computation, 2013, 9, 3505-3514.	2.3	7
97	Bio-Inspired Molecular Catalysts for Hydrogen Oxidation and Hydrogen Production. ACS Symposium Series, 2013, , 89-111.	0.5	7
98	Outer Coordination Sphere Proton Relay Base and Proximity Effects on Hydrogen Oxidation with Iron Electrocatalysts. Organometallics, 2019, 38, 1391-1396.	1.1	7
99	Thermal effects on the Clâ^'+ClCH2CN reaction by Car-Parrinello molecular dynamics. Journal of Chemical Physics, 2002, 117, 2199-2204.	1.2	6
100	Intramolecular solvation effects in the SN2 reaction Clâ^'+Cl(CH2)nCN. Journal of Chemical Physics, 2003, 119, 9063-9072.	1.2	6
101	Multi-scale modeling of HIV-1 proteins. Computational and Theoretical Chemistry, 2009, 898, 97-105.	1.5	6
102	Determinants of Selectivity for the Formation of Monocyclic and Bicyclic Products in Monoterpene Synthases. ACS Catalysis, 2022, 12, 7453-7469.	5.5	6
103	Weakening the Nâ€“H Bonds of NH₃ Ligands: Triple Hydrogen-Atom Abstraction to Form a Chromium(V) Nitride. Inorganic Chemistry, 2022, 61, 11165-11172.	1.9	6
104	Insights on the acetylated NFâ€ºB transcription factor complex with DNA from molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1560-1568.	1.5	5
105	Modulation of active site electronic structure by the protein matrix to control [NiFe] hydrogenase reactivity. Physical Chemistry Chemical Physics, 2014, 16, 24026-24033.	1.3	5
106	Splitting of multiple hydrogen molecules by bioinspired diniobium metal complexes: a DFT study. Dalton Transactions, 2021, 50, 840-849.	1.6	5
107	Quantitative Account of the Bonding Properties of a Rubredoxin Model Complex [Fe(SCH₃)₄]^q, q = â^'2, â^'1, +2, +3. Journal of Chemical Theory and Computation, 2021, 17, 6080-6091.	2.3	5
108	Changes in non-core regions stabilise plastocyanin from the thermophilic cyanobacterium Phormidium laminosum. Journal of Biological Inorganic Chemistry, 2010, 15, 329-338.	1.1	4

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109	Computational Investigations of the Reactivity of Metalloporphyrins for Ammonia Oxidation. Topics in Catalysis, 2022, 65, 341-353.	1.3	4
110	A molecular dynamics simulation of the vibrational properties of the Ar1âˆ'x(N2)x crystal. Journal of Chemical Physics, 1998, 109, 6382-6389.	1.2	3
111	Regioselectivity mechanism of the Thunbergia alata Î"6-16:0-acyl carrier protein desaturase. Plant Physiology, 2022, 188, 1537-1549.	2.3	3
112	Atomistic insight on structure and dynamics of spinach acyl carrier protein with substrate length. Biophysical Journal, 2021, 120, 3841-3853.	0.2	1
113	HIV-1 Integrase Binding to its Cellular Partners: A Perspective from Computational Biology. Current Pharmaceutical Design, 2014, 20, 3412-3421.	0.9	1
114	A novel parametrization scheme for classical and quantum mechanical simulations of large, floppy molecular systems. Chemical Physics Letters, 2006, 427, 230-235.	1.2	0
115	Inside Cover: The Role of Pendant Amines in the Breaking and Forming of Molecular Hydrogen Catalyzed by Nickel Complexes (Chem. Eur. J. 21/2012). Chemistry - A European Journal, 2012, 18, 6402-6402.	1.7	0
116	Protonation of Serine in Gas and Condensed and Microsolvated States in Aqueous Solution. Journal of Physical Chemistry A, 2022, 126, 44-52.	1.1	0