Sandra Luber

List of Publications by Year in Descending Order

83 papers	2,323 citations	27 h-index	46 g-index
92 ext. papers	2,610 ext. citations	5.1 avg, IF	5.68 L-index

#	Paper	IF	Citations
83	Closer Look at Inverse Electron Demand Diels-Alder and Nucleophilic Addition Reactions on -Tetrazines Using Enhanced Sampling Methods.. *Topics in Catalysis*, **2022**, 65, 1-17	2.3	1
82	The photodissociation of solvated cyclopropanone and its hydrate explored non-adiabatic molecular dynamics using SCF.. *Physical Chemistry Chemical Physics*, **2022**,	3.6	4
81	Machine Learning-Assisted Discovery of Hidden States in Expanded Free Energy Space.. *Journal of Physical Chemistry Letters*, **2022**, 1797-1805	6.4	3
80	The SCF method for non-adiabatic dynamics of systems in the liquid phase.. *Journal of Chemical Physics*, **2022**, 156, 130901	3.9	3
79	Robust SCF calculations with direct energy functional minimization methods and STEP for molecules and materials.. *Journal of Chemical Physics*, **2022**, 156, 154104	3.9	1
78	Local approaches for electric dipole moments in periodic systems and their application to real-time time-dependent density functional theory. *Journal of Chemical Physics*, **2021**, 155, 134116	3.9	2
77	Nucleophilic Attack on Nitrogen in Tetrazines by Silyl-Enol Ethers. *Organic Letters*, **2021**, 23, 2426-2430	6.2	6
76	How Molecular Dynamics Can Change the Understanding on Transition Metal Catalysed Water Oxidation. *Chimia*, **2021**, 75, 195-201	1.3	1
75	Analytic calculation and analysis of atomic polar tensors for molecules and materials using the Gaussian and plane waves approach. *Journal of Chemical Physics*, **2021**, 154, 104121	3.9	1
74	Fast Estimation of Mller-Plesset Correlation Energies Based on Atomic Contributions. *Journal of Physical Chemistry Letters*, **2021**, 12, 5324-5331	6.4	0
73	Time Domain Simulation of (Resonance) Raman Spectra of Liquids in the Short Time Approximation. *Journal of Chemical Theory and Computation*, **2021**, 17, 344-356	6.4	6
72	A Machine Learning Approach for MP2 Correlation Energies and Its Application to Organic Compounds. *Journal of Chemical Theory and Computation*, **2021**, 17, 777-790	6.4	3
71	SCF with Subsystem Density Embedding for Efficient Nonadiabatic Molecular Dynamics in Condensed-Phase Systems. *Journal of Chemical Theory and Computation*, **2021**, 17, 1653-1661	6.4	6
70	Water-Assisted Chemical Route Towards the Oxygen Evolution Reaction at the Hydrated (110) Ruthenium Oxide Surface: Heterogeneous Catalysis via DFT-MD and Metadynamics Simulations. *Chemistry - A European Journal*, **2021**, 27, 17024-17037	4.8	2
69	Explicit solvent effects on (1 1 0) ruthenium oxide surface wettability: Structural, electronic and mechanical properties of rutile RuO2 by means of spin-polarized DFT-MD. *Applied Surface Science*, **2021**, 570, 150993	6.7	6
68	Zooming in on the O-O Bond Formation-An Ab Initio Molecular Dynamics Study Applying Enhanced Sampling Techniques. *Journal of Chemical Theory and Computation*, **2020**, 16, 2436-2449	6.4	17
67	Trajectory Surface Hopping Nonadiabatic Molecular Dynamics with Kohn-Sham SCF for Condensed-Phase Systems. *Journal of Chemical Theory and Computation*, **2020**, 16, 4071-4086	6.4	13

66	Enhanced Ab Initio Molecular Dynamics Exploration Unveils the Complex Role of Different Intramolecular Bases on the Water Nucleophilic Attack Mechanism. *ACS Catalysis*, **2020**, 10, 7657-7667	13.1	11
65	Trajectory-based machine learning method and its application to molecular dynamics. *Molecular Physics*, **2020**, 118, e1788189	1.7	4
64	Electrochemically and Photochemically Induced Hydrogen Evolution Catalysis with Cobalt Tetraazamacrocycles Occurs Through Different Pathways. *ChemSusChem*, **2020**, 13, 2745-2752	8.3	6
63	Complete active space analysis of a reaction pathway: Investigation of the oxygen-oxygen bond formation. *Journal of Computational Chemistry*, **2020**, 41, 1586-1597	3.5	4
62	Investigating the Structure and Dynamics of Apo-Photosystem II. *ChemCatChem*, **2019**, 11, 4072-4080	5.2	3
61	Mechanistically Driven Control over Cubane Oxo Cluster Catalysts. *Journal of the American Chemical Society*, **2019**, 141, 8846-8857	16.4	15
60	Insights into artificial water oxidation: A computational perspective. *Advances in Inorganic Chemistry*, **2019**, 61-114	2.1	1
59	Electronic circular dichroism with real time time dependent density functional theory: Propagator formalism and gauge dependence. *Chemical Physics*, **2019**, 527, 110464	2.3	13
58	Determination of pKa Values via ab initio Molecular Dynamics and its Application to Transition Metal-Based Water Oxidation Catalysts. *Inorganics*, **2019**, 7, 73	2.9	16
57	Recent progress in computational exploration and design of functional materials. *Computational Materials Science*, **2019**, 161, 127-134	3.2	7
56	Trendbericht Theoretische Chemie: Schwingungsspektroskopie mit Ab-initio-Molekulardynamik. *Nachrichten Aus Der Chemie*, **2019**, 67, 61-64	0.1	
55	Vibrational (resonance) Raman optical activity with real time time dependent density functional theory. *Journal of Chemical Physics*, **2019**, 151, 234110	3.9	15
54	Computational Modeling of Cobalt-Based Water Oxidation: Current Status and Future Challenges. *Frontiers in Chemistry*, **2018**, 6, 100	5	30
53	Dynamic Methods for Vibrational Spectroscopy. *Chimia*, **2018**, 72, 328-332	1.3	2
52	Advancing Computational Approaches for Study and Design in Catalysis. *Chimia*, **2018**, 72, 508-513	1.3	2
51	Localized molecular orbitals for calculation and analysis of vibrational Raman optical activity. *Physical Chemistry Chemical Physics*, **2018**, 20, 28751-28758	3.6	6
50	Efficient calculation of (resonance) Raman spectra and excitation profiles with real-time propagation. *Journal of Chemical Physics*, **2018**, 149, 174108	3.9	14
49	Exploring the Limitation of Molecular Water Oxidation Catalysts. *Journal of Physical Chemistry C*, **2018**, 122, 12404-12412	3.8	27

48	Towards the rational design of the Py5-ligand framework for ruthenium-based water oxidation catalysts. *Dalton Transactions*, **2018**, 47, 10480-10490	4.3	10
47	Raman Optical Activity Spectra from Density Functional Perturbation Theory and Density-Functional-Theory-Based Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2017**, 13, 1254-1262	6.4	17
46	Dehydrogenation Free Energy of Co(aq) from Density Functional Theory-Based Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2017**, 13, 974-981	6.4	6
45	Exploring Solvation Effects in Ligand-Exchange Reactions via Static and Dynamic Methods. *Journal of Chemical Theory and Computation*, **2017**, 13, 3348-3358	6.4	15
44	Ruthenium Water Oxidation Catalysts based on Pentapyridyl Ligands. *ChemSusChem*, **2017**, 10, 4517-4525	8.3	20
43	{CoO} and {CoNiO} Cubane Water Oxidation Catalysts as Surface Cut-Outs of Cobalt Oxides. *Journal of the American Chemical Society*, **2017**, 139, 14198-14208	16.4	73
42	Discovery of Open Cubane Core Structures for Biomimetic LnCo (OR) Water Oxidation Catalysts. *ChemSusChem*, **2017**, 10, 4561-4569	8.3	13
41	Redox-Inert Cations Enhancing Water Oxidation Activity: The Crucial Role of Flexibility. *ACS Catalysis*, **2016**, 6, 6750-6761	13.1	30
40	Symmetry Breaking in Chiral Ionic Liquids Evidenced by Vibrational Optical Activity. *Angewandte Chemie - International Edition*, **2016**, 55, 11787-90	16.4	12
39	Ruthenium water oxidation catalysts containing the non-planar tetradentate ligand, biisoquinoline dicarboxylic acid (biqaH). *Dalton Transactions*, **2016**, 45, 19361-19367	4.3	21
38	Symmetriebruch in chiralen ionischen Flüssigkeiten: Nachweis durch vibratorisch-optische Aktivität. *Angewandte Chemie*, **2016**, 128, 11962-11966	3.6	1
37	What Influences the Water Oxidation Activity of a Bioinspired Molecular CoII4O4 Cubane? An In-Depth Exploration of Catalytic Pathways. *ACS Catalysis*, **2016**, 6, 1505-1517	13.1	50
36	Sum Frequency Generation of Acetonitrile on a Rutile (110) Surface from Density Functional Theory-Based Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2016**, 7, 5183-5187	6.4	15
35	Electronic communication in phosphine substituted bridged dirhenium complexes - clarifying ambiguities raised by the redox non-innocence of the C4H2- and C4-bridges. *Dalton Transactions*, **2016**, 45, 5783-99	4.3	15
34	Computational Investigation and Design of Cobalt Aqua Complexes for Homogeneous Water Oxidation. *Journal of Physical Chemistry C*, **2016**, 120, 7966-7975	3.8	31
33	Homogeneous Photochemical Water Oxidation with Cobalt Chloride in Acidic Media. *ACS Catalysis*, **2015**, 5, 4994-4999	13.1	19
32	Non-innocent adsorption of Co-pyrphyrin on rutile(110). *Physical Chemistry Chemical Physics*, **2015**, 17, 22846-54	3.6	18
31	3d-4f {Co(II)3Ln(OR)4} Cubanes as Bio-Inspired Water Oxidation Catalysts. *Journal of the American Chemical Society*, **2015**, 137, 11076-84	16.4	116

30	Exploring Raman optical activity for transition metals: From coordination compounds to solids. *Biomedical Spectroscopy and Imaging*, **2015**, 4, 255-268	1.3	9
29	EXAFS simulation refinement based on broken-symmetry DFT geometries for the Mn(IV)-Fe(III) center of class I RNR from Chlamydia trachomatis. *Dalton Transactions*, **2014**, 43, 576-83	4.3	3
28	Where does the Raman optical activity of [Rh(en)3](3+) come from? Insight from a combined experimental and theoretical approach. *Physical Chemistry Chemical Physics*, **2014**, 16, 23260-73	3.6	14
27	Structural Information on the Au Interface of Thiolate-Protected Gold Clusters: A Raman Spectroscopy Study. *Journal of Physical Chemistry C*, **2014**, 118, 9604-9611	3.8	93
26	Local electric dipole moments for periodic systems via density functional theory embedding. *Journal of Chemical Physics*, **2014**, 141, 234110	3.9	26
25	Raman spectra from ab initio molecular dynamics and its application to liquid S-methyloxirane. *Journal of Chemical Physics*, **2014**, 141, 094503	3.9	43
24	Closer to photosystem II: a Co4O4 cubane catalyst with flexible ligand architecture. *Journal of the American Chemical Society*, **2013**, 135, 18734-7	16.4	145
23	Solvent effects in calculated vibrational Raman optical activity spectra of helices. *Journal of Physical Chemistry A*, **2013**, 117, 2760-70	2.8	27
22	Photoinduced proton coupled electron transfer in 2-(2hydroxyphenyl)-benzothiazole. *Journal of Physical Chemistry A*, **2013**, 117, 5269-79	2.8	98
21	M(O)V(I)P(AC): vibrational spectroscopy with a robust meta-program for massively parallel standard and inverse calculations. *Journal of Computational Chemistry*, **2012**, 33, 2186-98	3.5	50
20	S1-state model of the O2-evolving complex of photosystem II. *Biochemistry*, **2011**, 50, 6308-11	3.2	196
19	Structural-functional role of chloride in photosystem II. *Biochemistry*, **2011**, 50, 6312-5	3.2	114
18	Ultrafast branching of reaction pathways in 2-(2hydroxyphenyl)benzothiazole in polar acetonitrile solution. *Journal of Physical Chemistry A*, **2011**, 115, 7550-8	2.8	63
17	Enhancement and de-enhancement effects in vibrational resonance Raman optical activity. *Journal of Chemical Physics*, **2010**, 132, 044113	3.9	50
16	Deciphering the role of RNA-binding proteins in the post-transcriptional control of gene expression. *Briefings in Functional Genomics*, **2010**, 9, 391-404	4.9	114
15	Theoretical Raman optical activity study of the beta domain of rat metallothionein. *Journal of Physical Chemistry B*, **2010**, 114, 1057-63	3.4	67
14	Prediction of Raman optical activity spectra of chiral 3-acetylcamphorato-cobalt complexes. *ChemPhysChem*, **2010**, 11, 1876-87	3.2	25
13	Intensity tracking for theoretical infrared spectroscopy of large molecules. *Journal of Chemical Physics*, **2009**, 130, 064105	3.9	35

12	Understanding the signatures of secondary-structure elements in proteins with Raman optical activity spectroscopy. *Chemistry - A European Journal*, **2009**, 15, 13491-508	4.8	65
11	Intensity-carrying modes in Raman and Raman optical activity spectroscopy. *ChemPhysChem*, **2009**, 10, 2049-57	3.2	37
10	On the direct calculation of the free energy of quantization for molecular systems in the condensed phase. *Journal of Computational Chemistry*, **2009**, 30, 514-23	3.5	6
9	Electromagnetic fields in relativistic one-particle equations. *Chemical Physics*, **2009**, 356, 205-218	2.3	22
8	Calculated Raman optical activity spectra of 1,6-anhydro-beta-D-glucopyranose. *Journal of Physical Chemistry A*, **2009**, 113, 8268-77	2.8	44
7	Analysis of secondary structure effects on the IR and Raman spectra of polypeptides in terms of localized vibrations. *Journal of Physical Chemistry B*, **2009**, 113, 6558-73	3.4	66
6	Intensity Tracking for Vibrational Spectra of Large Molecules. *Chimia*, **2009**, 63, 270-274	1.3	13
5	Relevance of the electric-dipole--electric-quadrupole contribution to Raman optical activity spectra. *Journal of Physical Chemistry B*, **2008**, 112, 2218-32	3.4	45
4	Calculated Raman optical activity signatures of tryptophan side chains. *ChemPhysChem*, **2008**, 9, 2177-80	3.2	48
3	Raman optical activity spectra of chiral transition metal complexes. *Chemical Physics*, **2008**, 346, 212-223	2.3	59
2	Recent Progress in the Simulation of Chiral Systems with Real Time Propagation Methods. *Helvetica Chimica Acta*,e2100154	2	2
1	Vibrational spectroscopy by means of first-principles molecular dynamics simulations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*,	7.9	5