Romuald Poteau

List of Publications by Year
in descending order

96	2,753	159358	205818
papers	citations	30 h-index	48 g-index

107	107	107	2940
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ruthenium Nanoparticles Stabilized by Nâ€Heterocyclic Carbenes: Ligand Location and Influence on Reactivity. Angewandte Chemie - International Edition, 2011, 50, 12080-12084.	7.2	199
2	Quantum chemistry-based interpretations on the lowest triplet state of luminescent lanthanides complexes. Part 1. Relation between the triplet state energy of hydroxamate complexes and their luminescence properties. Dalton Transactions, 2004, , 1334-1347.	1.6	146
3	Enantiospecific Cï£¿H Activation Using Ruthenium Nanocatalysts. Angewandte Chemie - International Edition, 2015, 54, 10474-10477.	7.2	118
4	Rare-Earth Metal Alkyl and Hydride Complexes Stabilized by a Cyclen-Derived [NNNN] Macrocyclic Ancillary Ligand. Journal of the American Chemical Society, 2008, 130, 6920-6921.	6.6	99
5	Theoretical and Experimental Studies on the Carbonâ€Nanotube Surface Oxidation by Nitric Acid: Interplay between Functionalization and Vacancy Enlargement. Chemistry - A European Journal, 2011, 17, 11467-11477.	1.7	93
6	Isomerisation and phase transitions in small sodium clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1994, 30, 57-68.	1.0	70
7	Ligand-Capped Ru Nanoparticles as Efficient Electrocatalyst for the Hydrogen Evolution Reaction. ACS Catalysis, 2018, 8, 11094-11102.	5.5	70
8	Structure, stability, and vibrational properties of small silver cluster. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1997, 40, 479-482.	1.0	66
9	Dimeric Gold Bis(carbene) Complexes by Transmetalation in Water. Organometallics, 2012, 31, 619-626.	1.1	65
10	Effective Group Potentials. 1. Method. Journal of Physical Chemistry A, 2001, 105, 198-205.	1.1	64
11	Structural properties of sodium microclusters (n=4â€“34) using a Monte Carlo growth method. Journal of Chemical Physics, 1993, 98, 6540-6557.	1.2	63
12	Calculation of the Electronic Spectrum of Li2 Using Effective Core Pseudopotentials and l -Dependent Core Polarization Potentials. Journal of Molecular Spectroscopy, 1995, 171, 299-308.	0.4	61
13	An ab initio study of mutual neutralization in Na++H-collisions. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, 5451-5461.	0.6	56
14	Distance-dependent HÃ¼ckel-type model for the study of sodium clusters. Physical Review B, 1992, 45, 1878-1888.	1.1	53
15	Evaluation of new thiadiazoles and benzothiazoles as potential radioprotectors: Free radical scavenging activity in vitro and theoretical studies (QSAR, DFT). Free Radical Biology and Medicine, 2009, 46, 1139-1148.	1.3	53
16	Synthesis and Reactivity of [Penta(4â€halogenophenyl)cyclopentadienyl][hydrotris(indazolyl)borato]ruthenium(II) Complexes: Rotationâ€Induced Fosbury Flop in an Organometallic Molecular Turnstile. Chemistry - A European Journal, 2008, 14, 8147-8156.	1.7	50
17	Zwitterionic amidinates as effective ligands for platinum nanoparticle hydrogenation catalysts. Chemical Science, 2017, 8, 2931-2941.	3.7	48
18	Theoretical Study of Ln(III) Complexes with Polyaza-Aromatic Ligands: Geometries of [LnL(H2O)n]3+Complexes and Successes and Failures of TD-DFT. Journal of Physical Chemistry A, 2005, 109, 4325-4330.	1.1	46

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19	Hydrido-Ruthenium Cluster Complexes as Models for Reactive Surface Hydrogen Species of Ruthenium Nanoparticles. Solid-State ²H NMR and Quantum Chemical Calculations. Journal of the American Chemical Society, 2010, 132, 11759-11767.	6.6	44
20	Theoretical characterization of the surface composition of ruthenium nanoparticles in equilibrium with syngas. Nanoscale, 2016, 8, 10974-10992.	2.8	43
21	All-cisCyclic Peptides. Journal of the American Chemical Society, 2005, 127, 13875-13889.	6.6	41
22	Spectroscopic and theoretical studies of the excited states of fenofibric acid and ketoprofen in relation with their photosensitizing properties. New Journal of Chemistry, 2000, 24, 403-410.	1.4	40
23	Ultrathin Gold Nanowires: Soft-Templating versus Liquid Phase Synthesis, a Quantitative Study. Journal of Physical Chemistry C, 2015, 119, 4422-4430.	1.5	40
24	DFT calculations of 1H and 13C NMR chemical shifts in transition metal hydrides. Dalton Transactions, 2008, , 3959.	1.6	37
25	Propensity for local folding induced by the urea fragment in short-chain oligomers. Organic and Biomolecular Chemistry, 2008, 6, 2596.	1.5	37
26	From Molecular Complexes to Complex Metallic Nanostructuresâ€"²H Solidâ€State NMR Studies of Rutheniumâ€Containing Hydrogenation Catalysts. ChemPhysChem, 2013, 14, 3026-3033.	1.0	37
27	Effective Group Potentials. 2. Extraction and Transferability for Chemical Groups Involved in Covalent or Donorâ"Acceptor Bonds. Journal of Physical Chemistry A, 2001, 105, 206-214.	1.1	31
28	Modeling C5H5with Atoms or Effective Group Potential in Lanthanide Complexes:Â Isolobality Not the Determining Factor. Journal of Physical Chemistry A, 2002, 106, 1797-1801.	1.1	31
29	Where does Hydrogen Adsorb on Ru Nanoparticles? A Powerful Joint ²H MASâ€NMR/DFT Approach. ChemPhysChem, 2009, 10, 2939-2942.	1.0	30
30	A Density Functional Theory Study of Spectroscopic and Thermodynamic Properties of Surfacic Hydrides on Ru (0001) Model Surface: The Influence of the Coordination Modes and the Coverage. Journal of Physical Chemistry C, 2011, 115, 2169-2178.	1.5	30
31	Grafting of Lanthanide Complexes on Silica Surfaces: A Theoretical Investigation. Journal of Physical Chemistry A, 2010, 114, 6322-6330.	1.1	29
32	Investigation of the surface chemistry of phosphine-stabilized ruthenium nanoparticles â€" an advanced solid-state NMR study. Physical Chemistry Chemical Physics, 2013, 15, 17383.	1.3	29
33	A new method for modelling spectator chemical groups in ab initio calculations: effective group potentials. Theoretical Chemistry Accounts, 2000, 104, 174-178.	0.5	25
34	Comparative studies of the spectroscopy of CuCl2: DFT versus standard ab initio approaches. Journal of Chemical Physics, 2005, 122, 164306.	1.2	24
35	DFT 2H quadrupolar coupling constants of ruthenium complexes: a good probe of the coordination of hydrides in conjuction with experiments. Physical Chemistry Chemical Physics, 2009, 11, 5657.	1.3	24
36	DFT study of the Ring Opening Polymerization of Îµ-caprolactone by grafted lanthanide complexes: 1â€"Effect of the grafting mode on the reactivity of borohydride complexes. Dalton Transactions, 2011, 40, 11211.	1.6	24

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37	Tin-decorated ruthenium nanoparticles: a way to tune selectivity in hydrogenation reaction. Nanoscale, 2014, 6, 9806-9816.	2.8	24
38	Quantum chemistry-based interpretations on the lowest triplet state of luminescent lanthanides complexes. Part 2. Influence of the electrostatic interactions on the triplet state energy of terbium complexes. Computational and Theoretical Chemistry, 2005, 756, 151-162.	1.5	23
39	DFT study of the Ring Opening Polymerization of Îµ-caprolactone by grafted lanthanide complexes: 2â€"Effect of the initiator ligand. Dalton Transactions, 2011, 40, 11228.	1.6	23
40	Amideâ€Functionalized Bis(NHC) Systems: Anion Effect on Goldâ€"Gold Interactions. European Journal of Inorganic Chemistry, 2012, 2012, 3892-3898.	1.0	23
41	Simple electron donor molecules based on triphenylamine and carbazole derivatives. Dyes and Pigments, 2018, 153, 275-283.	2.0	23
42	Hydrogen Isotope Exchange Catalyzed by Ru Nanocatalysts: Labelling of Complex Molecules Containing Nâ€Heterocycles and Reaction Mechanism Insights. Chemistry - A European Journal, 2020, 26, 4988-4996.	1.7	23
43	Ligand-Field Theory-Based Analysis of the Adsorption Properties of Ruthenium Nanoparticles. ACS Nano, 2013, 7, 9823-9835.	7.3	22
44	Surface-Engineering of Ultrathin Gold Nanowires: Tailored Self-Assembly and Enhanced Stability. Langmuir, 2017, 33, 5456-5463.	1.6	22
45	On the formation of transient (Na19)2 and (Na20)2 cluster dimers from molecular dynamics simulations. Physics Letters, Section A: General, Atomic and Solid State Physics, 1994, 193, 75-81.	0.9	21
46	Ultrathin Gold Nanowires with the Polytetrahedral Structure of Bulk Manganese. ACS Nano, 2018, 12, 9521-9531.	7.3	21
47	Ligand effect on the NMR, vibrational and structural properties of tetra- and hexanuclear ruthenium hydrido clusters: a theoretical investigation. Dalton Transactions, 2009, , 2142.	1.6	20
48	Dinuclear gold(I) and gold(III) complexes involving di(N-heterocyclic carbene) ligands â€" Synthesis, characterization and DFT studies. Journal of Organometallic Chemistry, 2013, 745-746, 242-250.	0.8	20
49	Effective group potentials: a powerful tool for hybrid QM/MM methods?. Computational and Theoretical Chemistry, 2003, 632, 43-59.	1.5	19
50	Carboxylic acid-capped ruthenium nanoparticles: experimental and theoretical case study with ethanoic acid. Nanoscale, 2019, 11, 9392-9409.	2.8	19
51	Catalysis to discriminate single atoms from subnanometric ruthenium particles in ultra-high loading catalysts. Catalysis Science and Technology, 2020, 10, 4673-4683.	2.1	18
52	Shape, electronic structure and steric effects of organometallic nanocatalysts: relevant tools to improve the synergy between theory and experiment. Dalton Transactions, 2017, 46, 378-395.	1.6	17
53	Yttrium Dihydride Cation [YH₂(THF)₂]⁺_n: Aggregate Formation and Reaction with (NNNN)-Type Macrocycles. Organometallics, 2015, 34, 3739-3747.	1.1	16
54	2H NMR calculations on polynuclear transition metal complexes: on the influence of local symmetry and other factors. Physical Chemistry Chemical Physics, 2011, 13, 20199.	1.3	15

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55	Grafting of lanthanide complexes on silica surfaces dehydroxylated at 200 Â°C: a theoretical investigation. New Journal of Chemistry, 2015, 39, 7703-7715.	1.4	15
56	Surprising Differences of Alkane Câ€H Activation Catalyzed by Ruthenium Nanoparticles: Complex Surfaceâ€Substrate Recognition?. ChemCatChem, 2018, 10, 4243-4247.	1.8	15
57	Chemical tuning of Coulomb blockade at room-temperature in ultra-small platinum nanoparticle self-assemblies. Materials Horizons, 2017, 4, 487-492.	6.4	14
58	Using Effective Group Potential Methodology for Predicting Organometallic Complex Properties. Journal of the American Chemical Society, 2003, 125, 11051-11061.	6.6	12
59	DFT calculations of 29Si-NMR chemical shifts in Ru(ii) silyl complexes: Searching for trends and accurate values. Dalton Transactions, 2011, 40, 11321.	1.6	12
60	Nanocatalysts for High Selectivity Enyne Cyclization: Oxidative Surface Reorganization of Gold Sub-2-nm Nanoparticle Networks. Jacs Au, 2021, 1, 187-200.	3.6	12
61	The effective group potential, a new method for the study of spectrum in large molecules: Tests and perspectives. Journal of Chemical Physics, 2002, 116, 4829.	1.2	11
62	The electronic spectrum of AgCl2: Ab initio benchmark versus density-functional theory calculations on the lowest ligand-field states including spin-orbit effects. Journal of Chemical Physics, 2006, 124, 034307.	1.2	11
63	Amphiphilic Organic Ion Pairs in Solution: A Theoretical Study. ChemPhysChem, 2007, 8, 1524-1533.	1.0	11
64	3D Ruthenium Nanoparticle Covalent Assemblies from Polymantane Ligands for Confined Catalysis. Chemistry of Materials, 2020, 32, 2365-2378.	3.2	11
65	Mo thio and oxo-thio molecular complexes film as self-healing catalyst for photocatalytic hydrogen evolution on 2D materials. Applied Catalysis B: Environmental, 2020, 278, 119288.	10.8	10
66	Global structure of small Na clusters in different approaches. Physics Letters, Section A: General, Atomic and Solid State Physics, 1998, 242, 163-168.	0.9	9
67	Ab initio molecular dynamics simulation of the UV absorption spectrum of Î²-ionone. Computational and Theoretical Chemistry, 2006, 771, 43-50.	1.5	9
68	A combined theoretical/experimental study highlighting the formation of carbides on Ru nanoparticles during CO hydrogenation. Nanoscale, 2021, 13, 6902-6915.	2.8	9
69	Bimetallic RuNi nanoparticles as catalysts for upgrading biomass: metal dilution and solvent effects on selectivity shifts. Green Chemistry, 2021, 23, 8480-8500.	4.6	9
70	Genetic algorithms for determining the topological structure of metallic clusters. European Physical Journal D, 1999, 9, 235-241.	0.6	8
71	What can we do with an effective group potential?. International Journal of Quantum Chemistry, 2006, 106, 727-733.	1.0	8
72	Estimating the â€œSteric Clashâ€•at cis Peptide Bonds. Journal of Physical Chemistry B, 2008, 112, 7894-7902.	1.2	8

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73	Surfaces of a Colloidal Iron Nanoparticle in Its Chemical Environment: A DFT Description. Langmuir, 2014, 30, 11670-11680.	1.6	8
74	Modeling a Carbonyl Group Taking into Account Back-Donation Effects through the Effective Group Potential Method. Journal of Physical Chemistry A, 2003, 107, 9393-9402.	1.1	7
75	Critical assessment of charge transfer estimates in non-covalent graphene doping. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	7
76	All-cisHelical Polypeptides. Journal of Organic Chemistry, 2007, 72, 8251-8258.	1.7	6
77	Absorption and solvatochromic properties of 2-methylisoindolin-1-one and related compounds: interplay between theory and experiments. New Journal of Chemistry, 2005, 29, 570.	1.4	5
78	Ruthenium Icosahedra and Ultrathin Platelets: The Role of Surface Chemistry on the Nanoparticle Structure. Chemistry of Materials, 2022, 34, 2931-2944.	3.2	5
79	Monte Carlo ab initio simulation of the absorption spectrum of Na4. Chemical Physics, 1993, 175, 289-297.	0.9	4
80	DFT calculations in periodic boundary conditions of gas-phase acidities and of transition-metal anionic clusters: case study with carboxylate-stabilized ruthenium clusters. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	4
81	Blue wine, a color obtained with synthetic blue dye addition: two case studies. European Food Research and Technology, 2019, 245, 1777-1782.	1.6	4
82	When organophosphorus ruthenium complexes covalently bind to ruthenium nanoparticles to form nanoscale hybrid materials. Chemical Communications, 2020, 56, 4059-4062.	2.2	3
83	Surface reactions of ammonia on ruthenium nanoparticles revealed by¹⁵N and¹³C solid-state NMR. Catalysis Science and Technology, 2021, 11, 4509-4520.	2.1	3
84	Correlation between surface chemistry and magnetism in iron nanoparticles. Nanoscale Advances, 2021, 3, 4471-4481.	2.2	3
85	Theoretical proposal for an organometallic route to cis-peptides. New Journal of Chemistry, 2009, 33, 1833.	1.4	2
86	Multicentered effective group potentials: ligand-field effects in organometallic clusters and dynamical study of chemical reactivity. Theoretical Chemistry Accounts, 2010, 126, 151-163.	0.5	2
87	How CuI and NaI Interact with Faujasite Zeolite? A Theoretical Investigation. Journal of Physical Chemistry C, 2020, 124, 28026-28037.	1.5	2
88	Structure, stability, and vibrational properties of small silver cluster. , 1997, , 479-482.		2
89	Supramolecular nanocapsules as two-fold stabilizers of outer-cavity sub-nanometric Ru NPs and inner-cavity ultra-small Ru clusters. Nanoscale Horizons, 2022, 7, 607-615.	4.1	2
90	Static, statistical, and dynamical properties of small sodium clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 232-235.	1.0	1

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91	Inside Cover: Theoretical and Experimental Studies on the Carbon-Nanotube Surface Oxidation by Nitric Acid: Interplay between Functionalization and Vacancy Enlargement (Chem. Eur. J. 41/2011). Chemistry - A European Journal, 2011, 17, 11354-11354.	1.7	1
92	Recent Progress in Atomic and Chemical Group Effective Potentials. Journal of Chemical Information and Computer Sciences, 2001, 41, 43-49.	2.8	0
93	Progress Towards a Rotary Molecular Motor. AIP Conference Proceedings, 2004, , .	0.3	0
94	Effective Group Potentials: A Powerful Tool for Hybrid QM/MM Methods?. ChemInform, 2004, 35, no.	0.1	0
95	Tuning Coulomb blockade in ultra-small metallic nanoparticle self-assemblies, at room-temperature. , 2016, , .		0
96	Recognition of the three-dimensional structure of small metal nanoparticles by a supervised artificial neural network. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	0