Emilia Sicilia

List of Publications by Year in Descending Order

122 papers	2,471 citations	29 h-index	42 g-index
129 ext. papers	2,819 ext. citations	4.7 avg, IF	5.2 L-index

#	Paper	IF	Citations
122	Computational Studies of the Photogeneration from Dihydrosanguinarine and the Probable Cytotoxicity Mechanism of Sanguinarine. *Applied Sciences (Switzerland)*, **2022**, 12, 1095	2.6	
121	Experimental and theoretical study of the complexation of Fe3+ and Cu2+ by l-ascorbic acid in aqueous solution. *Journal of Molecular Liquids*, **2022**, 355, 118973	6	0
120	Exploring the Structure-Performance Relationship of Sulfonated Polysulfone Proton Exchange Membrane by a Combined Computational and Experimental Approach. *Polymers*, **2021**, 13,	4.5	3
119	Is the cytotoxic activity of phenanthriplatin dependent on the specific size of the phenanthridine ligand system?. *Journal of Inorganic Biochemistry*, **2021**, 219, 111447	4.2	4
118	Anticancer Activity, DNA Binding, and Photodynamic Properties of a N?C?N-Coordinated Pt(II) Complex. *Inorganic Chemistry*, **2021**, 60, 10350-10360	5.1	5
117	Novel choline selective electrochemical membrane sensor with application in milk powders and infant formulas. *Talanta*, **2021**, 221, 121409	6.2	8
116	Betaine host-guest complexation with a calixarene receptor: enhanced anticancer effect.. *RSC Advances*, **2021**, 11, 24673-24680	3.7	4
115	A Boron-Containing Compound Acting on Multiple Targets Against Alzheimer's Disease. Insights from Ab Initio and Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling*, **2021**, 61, 3397-3410	6.1	6
114	Computational Analysis of Photophysical Properties and Reactivity of a New Phototherapeutic Cyclometalated Au(III)-Hydride Complex. *Chemistry - A European Journal*, **2021**, 27, 15528-15535	4.8	1
113	Cyclopentadienone NHC iron(0) complexes as low valent electrocatalysts for water oxidation. *Catalysis Science and Technology*, **2021**, 11, 1407-1418	5.5	1
112	Iodido equatorial ligands influence on the mechanism of action of Pt(IV) and Pt(II) anti-cancer complexes: A DFT computational study. *Journal of Computational Chemistry*, **2021**, 42, 608-619	3.5	1
111	Totally green cellulose conversion into bio-oil and cellulose citrate using molten citric acid in an open system: synthesis, characterization and computational investigation of reaction mechanisms.. *RSC Advances*, **2020**, 10, 34738-34751	3.7	11
110	Ligand-centred redox activation of inert organoiridium anticancer catalysts. *Chemical Science*, **2020**, 11, 5466-5480	9.4	14
109	Mechanism of action of the curcumin cis-diammineplatinum(II) complex as a photocytotoxic agent. *Inorganic Chemistry Frontiers*, **2020**, 7, 2759-2769	6.8	3
108	A metadynamics perspective on the reduction mechanism of the Pt(IV) asplatin prodrug. *Journal of Computational Chemistry*, **2020**, 41, 290-294	3.5	0
107	Rationalization of the Superior Anticancer Activity of Phenanthriplatin: An In-Depth Computational Exploration. *Chemistry - A European Journal*, **2020**, 26, 259-268	4.8	8
106	A comparative computational mechanistic study on derivatives of pyriplatin, modified with the CH2Ph3P+ group, as anticancer complexes targeting mitochondria. *Inorganica Chimica Acta*, **2020**, 512, 119863	2.7	1

105	Experimental and Computational Investigations of Carboplatin Supramolecular Complexes. *ACS Omega*, **2020**, 5, 31456-31466	3.9	10
104	Sequestering Ability of a Synthetic Chelating Agent towards Copper(II) and Iron(III): A Detailed Theoretical and Experimental Analysis. *Chemistry - an Asian Journal*, **2020**, 15, 3266-3274	4.5	2
103	Theoretical exploration of the photophysical properties of two-component Ru-porphyrin dyes as promising assemblies for a combined antitumor effect. *Dalton Transactions*, **2020**, 49, 12653-12661	4.3	2
102	Host-Guest Complexation of Oxaliplatin and Sulfonatocalix[n]Arenes for Potential Use in Cancer Therapy. *Molecules*, **2020**, 25,	4.8	9
101	A multi-methodological inquiry of the behavior of cisplatin-based Pt(IV) derivatives in the presence of bioreductants with a focus on the isolated encounter complexes. *Journal of Biological Inorganic Chemistry*, **2020**, 25, 655-670	3.7	10
100	The Onset of Dehydrogenation in Solid Ammonia Borane: An Ab Initio Metadynamics Study. *Angewandte Chemie - International Edition*, **2019**, 58, 3976-3980	16.4	17
99	Spectrophotometric determination of choline in pharmaceutical formulations via host-guest complexation with a biomimetic calixarene receptor. *Microchemical Journal*, **2019**, 146, 735-741	4.8	7
98	Theoretical exploration of the reduction reaction of monofunctional phenanthriplatin Pt(IV) prodrugs. *Inorganica Chimica Acta*, **2019**, 495, 118951	2.7	0
97	Rational Design of Modified Oxobacteriochlorins as Potential Photodynamic Therapy Photosensitizers. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	5
96	Antitumor Platinium(IV) Prodrugs: A Systematic Computational Exploration of Their Reduction Mechanism by l-Ascorbic Acid. *Inorganic Chemistry*, **2019**, 58, 3851-3860	5.1	13
95	Structures, binding energies, temperature effects, infrared spectroscopy of [Mg(NH)] clusters from DFT and MP2 investigations. *Journal of Computational Chemistry*, **2019**, 40, 1707-1717	3.5	11
94	Elusive Intermediates in the Breakdown Reactivity Patterns of Prodrug Platinum(IV) Complexes. *Journal of the American Society for Mass Spectrometry*, **2019**, 30, 1881-1894	3.5	6
93	Blind Search for Complex Chemical Pathways Using Harmonic Linear Discriminant Analysis. *Journal of Chemical Theory and Computation*, **2019**, 15, 4507-4515	6.4	13
92	Photophysical Exploration of Dual-Approach Pt-BODIPY Conjugates: Theoretical Insights. *Inorganic Chemistry*, **2019**, 58, 9882-9889	5.1	10
91	A study on the physicochemical properties and cytotoxic activity of p-sulfocalix[4]arene-nedaplatin complex. *Journal of Physics: Conference Series*, **2019**, 1310, 012011	0.3	6
90	The role of the halogen bond in iodothyronine deiodinase: Dependence on chalcogen substitution in naphthyl-based mimetics. *Journal of Computational Chemistry*, **2019**, 40, 944-951	3.5	10
89	The Onset of Dehydrogenation in Solid Ammonia Borane: An Ab Initio Metadynamics Study. *Angewandte Chemie*, **2019**, 131, 4016-4020	3.6	7
88	Glutathione activation of an organometallic half-sandwich anticancer drug candidate by ligand attack. *Chemical Communications*, **2019**, 55, 14602-14605	5.8	14

87	Theoretical insight into joint photodynamic action of a gold(i) complex and a BODIPY chromophore for singlet oxygen generation. *Physical Chemistry Chemical Physics*, **2019**, 21, 3446-3452	3.6	5
86	Computational Investigation of the Influence of Halogen Atoms on the Photophysical Properties of Tetraphenylporphyrin and Its Zinc(II) Complexes. *Journal of Physical Chemistry A*, **2018**, 122, 2809-2815	2.8	11
85	Quantum mechanical DFT elucidation of CO2 catalytic conversion mechanisms: Three examples. *International Journal of Quantum Chemistry*, **2018**, 118, e25572	2.1	9
84	B,N-Codoped graphene as catalyst for the oxygen reduction reaction: Insights from periodic and cluster DFT calculations. *Journal of Computational Chemistry*, **2018**, 39, 637-647	3.5	32
83	Investigation of the host-guest complexation between 4-sulfocalix[4]arene and nedaplatin for potential use in drug delivery. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy* , **2018**, 193, 528-536	4.4	30
82	Excitation energies, singlet-triplet energy gaps, spin-orbit matrix elements and heavy atom effects in BOIMPYs as possible photosensitizers for photodynamic therapy: a computational investigation. *Physical Chemistry Chemical Physics*, **2018**, 20, 2656-2661	3.6	15
81	Insights from Computations on the Mechanism of Reduction by Ascorbic Acid of Pt Prodrugs with Asplatin and Its Chlorido and Bromido Analogues as Model Systems. *Chemistry - A European Journal*, **2018**, 24, 9572-9580	4.8	10
80	BODIPY for photodynamic therapy applications: computational study of the effect of bromine substitution on O photosensitization. *Journal of Molecular Modeling*, **2018**, 24, 183	2	8
79	Anionic cyclometalated Pt(ii) and Pt(iv) complexes respectively bearing one or two 1,2-benzenedithiolate ligands. *Dalton Transactions*, **2018**, 47, 11645-11657	4.3	7
78	Theoretical determination of the aquation reaction mechanism of cyclometalated benzimidazole Ru(II) and Ir(III) anticancer complexes. *Inorganica Chimica Acta*, **2018**, 470, 325-330	2.7	2
77	Can BODIPY Dimers Act as Photosensitizers in Photodynamic Therapy? A Theoretical Prediction. *Frontiers in Physics*, **2018**, 6,	3.9	8
76	Experimental and Theoretical Investigation on the Catalytic Generation of Environmentally Persistent Free Radicals from Benzene. *Journal of Physical Chemistry C*, **2017**, 121, 9381-9393	3.8	24
75	Hydrolysis in Acidic Environment and Degradation of Satraplatin: A Joint Experimental and Theoretical Investigation. *Inorganic Chemistry*, **2017**, 56, 6013-6026	5.1	8
74	Direct and cluster-assisted dehydrogenation of methane by Nb and Ta: a theoretical investigation. *Physical Chemistry Chemical Physics*, **2017**, 19, 16178-16188	3.6	5
73	Complexation of Al and Ni by l-Ascorbic Acid: An Experimental and Theoretical Investigation. *Journal of Physical Chemistry A*, **2017**, 121, 9773-9781	2.8	13
72	Metal Atom Effect on the Photophysical Properties of Mg(II), Zn(II), Cd(II), and Pd(II) Tetraphenylporphyrin Complexes Proposed as Possible Drugs in Photodynamic Therapy. *Molecules*, **2017**, 22,	4.8	34
71	A DFT investigation of a bulky biomimetic model catalyzing the 5'-outer ring deiodination of thyroxine. *Journal of Molecular Modeling*, **2016**, 22, 287	2	2
70	Computational Insight on CO2 Fixation to Produce Styrene Carbonate Assisted by a Single-Center Aluminum(III) Catalyst and Quaternary Ammonium Salts. *ChemCatChem*, **2016**, 8, 1167-1175	5.2	17

69	Investigation of the Inertness to Hydrolysis of Platinum(IV) Prodrugs. *Inorganic Chemistry*, **2016**, 55, 1580-6	5.1	24
68	Computation modeling as a tool for the exploration of complex multistep reaction cycles in homogeneous catalysis. Some selected examples in the framework of the use of hydrogen as a fuel of the future. *International Journal of Quantum Chemistry*, **2016**, 116, 1507-1512	2.1	1
67	Catalytic role of dinuclear μ-acetylide gold(I) complexes in the hydroamination of terminal alkynes: theoretical insights. *Journal of Chemical Theory and Computation*, **2015**, 11, 581-90	6.4	16
66	Mass Spectrometric and Computational Investigation of the Protonated Carnosine-Carboplatin Complex Fragmentation. *Inorganic Chemistry*, **2015**, 54, 7885-97	5.1	3
65	Collision-induced dissociation products of the protonated dipeptide carnosine: structural elucidation, fragmentation pathways and potential energy surface analysis. *Physical Chemistry Chemical Physics*, **2015**, 17, 12673-82	3.6	5
64	DFT Investigation of the Mechanism of Action of Organoiridium(III) Complexes As Anticancer Agents. *Inorganic Chemistry*, **2015**, 54, 10801-10	5.1	23
63	The heavy atom effect on Zn(ii) phthalocyanine derivatives: a theoretical exploration of the photophysical properties. *Physical Chemistry Chemical Physics*, **2015**, 17, 23595-601	3.6	41
62	Mechanism of thyroxine deiodination by naphthyl-based iodothyronine deiodinase mimics and the halogen bonding role: a DFT investigation. *Chemistry - A European Journal*, **2015**, 21, 8554-60	4.8	7
61	Ab initio calculations on the (1)O2 quenching mechanism by trans-resveratrol. *Physical Chemistry Chemical Physics*, **2014**, 16, 12773-81	3.6	11
60	Electronic spectra and intersystem spin-orbit coupling in 1,2- and 1,3-squaraines. *Journal of Computational Chemistry*, **2014**, 35, 2107-13	3.5	30
59	Oxidation of Ethylbenzene to Acetophenone with N-Doped Graphene: Insight from Theory. *Journal of Physical Chemistry C*, **2014**, 118, 12275-12284	3.8	31
58	The Role of Chelating Phosphine Rhodium Complexes in Dehydrocoupling Reactions of Amine-Boranes: A Theoretical Investigation Attempting To Rationalize the Observed Behaviors. *ACS Catalysis*, **2014**, 4, 1104-1113	13.1	18
57	Hydrogen release from dialkylamine-boranes promoted by Mg and Ca complexes: a DFT analysis of the reaction mechanism. *Chemistry - A European Journal*, **2014**, 20, 5967-76	4.8	20
56	Theoretical investigation of the absorption spectra and singlet-triplet energy gap of positively charged tetraphenylporphyrins as potential photodynamic therapy photosensitizers. *Canadian Journal of Chemistry*, **2013**, 91, 902-906	0.9	20
55	Hydrophilic annulated dinuclear zinc(II) phthalocyanine as Type II photosensitizers for PDT: a combined experimental and (TD)-DFT investigation. *Journal of Porphyrins and Phthalocyanines*, **2013**, 17, 980-988	1.8	8
54	EH3 (E = N, P, As) and H2 activation with N-heterocyclic silylene and germylene homologues. *Chemistry - A European Journal*, **2013**, 19, 7835-46	4.8	25
53	A time-dependent density functional study of a non-aromatic [1.1.1.1.1]-pentaphyrin and its lutetium complex. *Journal of Physical Chemistry B*, **2012**, 116, 10816-23	3.4	16
52	The performance of density functional based methods in the description of selected biological systems and processes. *Physical Chemistry Chemical Physics*, **2012**, 14, 14943-53	3.6	27

51	Homogeneous Gold Catalysis: Hydration of 1,2-Diphenylacetylene with Methanol in Aqueous Media. A Theoretical Viewpoint. *Organometallics*, **2012**, 31, 3074-3080	3.8	39
50	Dimethylplatinum(II) complexes: computational insights into Pt-C bond protonolysis. *Inorganic Chemistry*, **2011**, 50, 10091-101	5.1	21
49	Do rhodium bis(□amine-borane) complexes play a role as intermediates in dehydrocoupling reactions of amine-boranes?. *Chemistry - A European Journal*, **2011**, 17, 14586-92	4.8	14
48	Mechanistic insight into protonolysis and cis-trans isomerization of benzylplatinum(II) complexes assisted by weak ligand-to-metal interactions. A combined kinetic and DFT study. *Inorganic Chemistry*, **2011**, 50, 2224-39	5.1	14
47	Gold(I)-Catalyzed Hydration of 1,2-Diphenylacetylene: Computational Insights. *Journal of Chemical Theory and Computation*, **2010**, 6, 2782-9	6.4	16
46	Computational study of alkynes insertion into metal-hydride bonds catalyzed by bimetallic complexes. *Inorganic Chemistry*, **2010**, 49, 9875-83	5.1	17
45	Mechanistic investigation of the hydrogenation of O(2) by a transfer hydrogenation catalyst. *Journal of the American Chemical Society*, **2010**, 132, 4178-90	16.4	32
44	The influence of surface oxygen and hydroxyl groups on the dehydrogenation of ethylene on PdAu surface alloys. A theoretical cluster model study. *Chemical Physics Letters*, **2010**, 493, 87-93	2.5	5
43	Adsorption of Ethylene, Vinyl, Acetic Acid, and Acetate Species on PdAu(111) and PdAu(100) Surface Alloys: A Cluster Model Study. *Journal of Chemical Theory and Computation*, **2009**, 5, 1350-60	6.4	23
42	Can phthalocyanines and their substituted alpha-para-(methoxy)phenyl derivatives act as photosensitizers in photodynamic therapy? A TD-DFT study. *Physical Chemistry Chemical Physics*, **2009**, 11, 4586-92	3.6	20
41	On the Potential Use of Squaraine Derivatives as Photosensitizers in Photodynamic Therapy: A TDDFT and RICC2 Survey. *Journal of Chemical Theory and Computation*, **2009**, 5, 1849-57	6.4	40
40	Can subpyriporphyrin and its boron complex be proposed as photosensitizers in photodynamic therapy ? A first principle time dependent study. *Photochemical and Photobiological Sciences*, **2009**, 8, 386-90	4.2	8
39	First-principle time-dependent study of magnesium-containing porphyrin-like compounds potentially useful for their application in photodynamic therapy. *Journal of Physical Chemistry B*, **2008**, 112, 4123-30	3.4	47
38	On the Nature of the CP Bond in Phosphaalkynes. *Journal of Chemical Theory and Computation*, **2008**, 4, 397-403	6.4	13
37	Interaction of CO with PdAu(111) and PdAu(100) Bimetallic Surfaces: A Theoretical Cluster Model Study. *Journal of Physical Chemistry C*, **2008**, 112, 6073-6081	3.8	35
36	Theoretical Investigation of the Mechanism of Acid-Catalyzed Oxygenation of a Pd(II)-Hydride To Produce a Pd(II)-Hydroperoxide. *Journal of Chemical Theory and Computation*, **2008**, 4, 1283-92	6.4	21
35	Mechanistic aspects of the reaction of Th+ and Th2+ with water in the gas phase. *Inorganic Chemistry*, **2008**, 47, 2083-8	5.1	30
34	Hydration of ionic species studied by the reference interaction site model with a repulsive bridge correction. *Journal of Computational Chemistry*, **2008**, 29, 2406-15	3.5	38

33	The recognition of a new pathway for the reaction of molecular oxygen with a Pd(II)-hydride to produce a Pd(II)-hydroperoxide. *Chemical Physics Letters*, **2008**, 456, 41-46	2.5	15
32	beta-Hydrogen Kinetic Effect. *Journal of the American Chemical Society*, **2007**, 129, 5744-55	16.4	27
31	Gas-phase chemistry of actinides ions: new insights into the reaction of UO+ and UO2+ with water. *Journal of the American Chemical Society*, **2007**, 129, 4229-39	16.4	67
30	Absorption Spectra of the Potential Photodynamic Therapy Photosensitizers Texaphyrins Complexes: A Theoretical Analysis. *Journal of Chemical Theory and Computation*, **2007**, 3, 860-9	6.4	34
29	On the insertion mechanism of molecular oxygen into a Pd(II)H bond. Something to add. *Chemical Physics Letters*, **2007**, 443, 183-189	2.5	24
28	The role of quantum chemistry in the elucidation of the elementary mechanisms of catalytic processes: from atoms, to surfaces, to enzymes. *Theoretical Chemistry Accounts*, **2007**, 117, 765-779	1.9	36
27	Structures and electronic absorption spectra of a recently synthesised class of photodynamic therapy agents. *Chemistry - A European Journal*, **2006**, 12, 6797-803	4.8	94
26	Methane activation by chromium oxide cations in the gas phase: a theoretical study. *Journal of Computational Chemistry*, **2006**, 27, 174-87	3.5	30
25	Activation of methane by the iron dimer cation. A theoretical study. *Journal of Physical Chemistry A*, **2006**, 110, 12501-11	2.8	23
24	A theoretical study of ethylene dehydrogenation by bare Niobium atom and cation. *Computational and Theoretical Chemistry*, **2006**, 762, 25-31		14
23	Solvation properties of N-substituted cis and trans amides are not identical: significant enthalpy and entropy changes are revealed by the use of variable temperature 1H NMR in aqueous and chloroform solutions and ab initio calculations. *Journal of Physical Chemistry A*, **2005**, 109, 11878-84	2.8	16
22	About the Mulliken electronegativity in DFT. *Theoretical Chemistry Accounts*, **2005**, 114, 38-45	1.9	81
21	Acetylene cyclotrimerization by early second-row transition metals in the gas phase. A theoretical study. *Inorganic Chemistry*, **2005**, 44, 9807-16	5.1	26
20	On the applicability of the HSAB principle through the use of improved computational schemes for chemical hardness evaluation. *Journal of Computational Chemistry*, **2004**, 25, 994-1003	3.5	53
19	Structures, harmonic vibrational frequencies and interconversion potential energy profile of Ni+(C2H2)2 complexes. *Computational and Theoretical Chemistry*, **2004**, 709, 167-170		6
18	Combined molecular mechanics, molecular dynamics and quantum mechanical study of (+)-multifidene structure and conformation. *Chemistry and Ecology*, **2004**, 20, 157-165	2.3	
17	Theoretical Study of Two-State Reactivity of Transition Metal Cations: The Difficult Case of Iron Ion Interacting with Water, Ammonia, and Methane. *Journal of Physical Chemistry A*, **2004**, 108, 1069-1081	2.8	106
16	Density functional study of ammonia activation by late first-row transition metal cations. *Inorganic Chemistry*, **2004**, 43, 4944-52	5.1	34

15	Structure and Coordination Modes in the Interaction between Cd2+ and 3-Mercaptopropionic Acid. *Journal of Physical Chemistry A*, **2004**, 108, 8407-8410	2.8	15
14	The electronic states of Fe2+. *Chemical Physics Letters*, **2003**, 376, 310-317	2.5	18
13	Topological Analysis of the Reaction of Mn+ (7S,5S) with H2O, NH3, and CH4 Molecules. *Journal of Physical Chemistry A*, **2003**, 107, 4862-4868	2.8	62
12	Reaction of bare VO+ and FeO+ with ammonia: a theoretical point of view. *Inorganic Chemistry*, **2003**, 42, 8773-82	5.1	26
11	Atomic Radii Scale and Related Size Properties from Density Functional Electronegativity Formulation. *Journal of Physical Chemistry A*, **2003**, 107, 5461-5465	2.8	53
10	On the interaction between manganese cation (Mn2+) and the nucleic acid bases (T, U, C, A, G) in the gas phase. *International Journal of Quantum Chemistry*, **2002**, 90, 903-909	2.1	32
9	Theoretical study of ammonia and methane activation by first-row transition metal cations M(+) (M = Ti, V, Cr). *Journal of the American Chemical Society*, **2002**, 124, 1471-80	16.4	89
8	Insertion Reaction of Mn+ Bare Metal Cation into the NH and CH Bonds of Ammonia and Methane. *Journal of Physical Chemistry A*, **2002**, 106, 8937-8944	2.8	43
7	Reaction of SC+(1D,3D) with H2O, NH3, and CH4: a density functional study. *Journal of the American Chemical Society*, **2001**, 123, 2588-96	16.4	90
6	Density functional potential-energy hypersurface and reactivity indices in the isomerization of X3H+ (X = O, S, Se, Te). *Journal of the Chemical Society, Faraday Transactions*, **1997**, 93, 3309-3312		17
5	Molecular quadrupole moments, second moments, and diamagnetic susceptibilities evaluated using the generalized gradient approximation in the framework of Gaussian density functional method. *Journal of Chemical Physics*, **1996**, 105, 3206-3210	3.9	24
4	Geometries, singlet-triplet separations, dipole moments, ionization potentials, and vibrational frequencies in methylene (CH2) and halocarbenes (CHF, CF2, CCl2, CBr2, and CI2). *Journal of Chemical Physics*, **1992**, 97, 5031-5036	3.9	80
3	Conformation and structure of ethane-1,2-dithiol from ab initio HF and MP3 study. *Computational and Theoretical Chemistry*, **1992**, 257, 485-490		4
2	Two State Reactivity Paradigm in Catalysis. The Example of X?H (X = O, N, C) and C?C Bonds Activation Mediated by Transition Metal Compounds337-366		
1	A novel catalytic two-step process for the preparation of rigid polyurethane foams: synthesis, mechanism and computational studies. *Reaction Chemistry and Engineering*,	4.9	4