Federico Palazzetti

List of Publications by Year
in descending order

84	1,678	201575 27	315616 38
papers	citations	h-index	g-index

85	85	85	889
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	TD-DFT Benchmark on Inorganic Pt(II) and Ir(III) Complexes. Journal of Chemical Theory and Computation, 2015, 11, 3281-3289.	2.3	104
2	The Hydrogen Peroxideâ˜'Rare Gas Systems:Â Quantum Chemical Calculations and Hyperspherical Harmonic Representation of the Potential Energy Surface for Atomâ˜'Floppy Molecule Interactionsâ€. Journal of Physical Chemistry A, 2007, 111, 12754-12762.	1.1	72
3	A quantum chemical study of H2S2: Intramolecular torsional mode and intermolecular interactions with rare gases. Journal of Chemical Physics, 2008, 129, 164302.	1.2	60
4	Simulation of oriented collision dynamics of simple chiral molecules. International Journal of Quantum Chemistry, 2011, 111, 1651-1658.	1.0	55
5	Quantum Chemistry of C₃H₆O Molecules: Structure and Stability, Isomerization Pathways, and Chirality Changing Mechanisms. Journal of Physical Chemistry A, 2010, 114, 9864-9874.	1.1	49
6	Electrostatic Hexapole State-Selection of the Asymmetric-Top Molecule Propylene Oxide. Journal of Physical Chemistry A, 2010, 114, 3280-3286.	1.1	48
7	Spherical and hyperspherical representation of potential energy surfaces for intermolecular interactions. International Journal of Quantum Chemistry, 2011, 111, 318-332.	1.0	48
8	Potential energy surfaces for interactions of H2O with H2, N2 and O2: A hyperspherical harmonics representation, and a minimal model for the H2Oâ€"rare-gas-atom systems. Computational and Theoretical Chemistry, 2012, 990, 53-61.	1.1	47
9	Advances in non-equilibrium $$\hbox {CO}_2$$ plasma kinetics: a theoretical and experimental review. European Physical Journal D, 2021, 75, 1.	0.6	47
10	Range and strength of intermolecular forces for van der Waals complexes of the type H₂X_nâ€Rg, with X = O, S and n = 1,2. International Journal of Quantum Chemistry, 2010, 110, 777-786.	1.0	46
11	High-Accuracy Vibrational Computations for Transition-Metal Complexes Including Anharmonic Corrections: Ferrocene, Ruthenocene, and Osmocene as Test Cases. Journal of Chemical Theory and Computation, 2014, 10, 4565-4573.	2.3	46
12	Roads leading to roam. Role of triple fragmentation and of conical intersections in photochemical reactions: experiments and theory on methyl formate. Physical Chemistry Chemical Physics, 2014, 16, 2854-2865.	1.3	45
13	Aligned molecular collisions and a stereodynamical mechanism for selective chirality. Rendiconti Lincei, 2011, 22, 125-135.	1.0	44
14	The origin of chiral discrimination: supersonic molecular beam experiments and molecular dynamics simulations of collisional mechanisms. Physica Scripta, 2008, 78, 058119.	1.2	43
15	Aligned molecules: chirality discrimination in photodissociation and in molecular dynamics. Rendiconti Lincei, 2013, 24, 299-308.	1.0	43
16	Electrostatic hexapole state-selection of the asymmetric-top molecule propylene oxide: Rotational and orientational distributions. Chemical Physics, 2012, 399, 180-192.	0.9	41
17	A comparison of interatomic potentials for rare gas nanoaggregates. Computational and Theoretical Chemistry, 2008, 852, 22-29.	1.5	40
18	Alignment and Chirality in Gaseous Flows. Journal of the Vacuum Society of Japan, 2010, 53, 645-653.	0.3	38

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19	Hyperspherical representation of potential energy surfaces: intermolecular interactions in tetra-atomic and penta-atomic systems. Physica Scripta, 2011, 84, 028111.	1.2	38
20	Collisional autoionization dynamics of Neâˆ—(3P2,0)â€“H2O. Chemical Physics Letters, 2012, 546, 34-39.	1.2	38
21	Dynamical, spectroscopic and computational imaging of bond breaking in photodissociation: roaming and role of conical intersections. Faraday Discussions, 2015, 177, 77-98.	1.6	37
22	Directions of chemical change: experimental characterization of the stereodynamics of photodissociation and reactive processes. Physical Chemistry Chemical Physics, 2014, 16, 9776.	1.3	36
23	Molecular alignment and chirality in gaseous streams and vortices. Rendiconti Lincei, 2013, 24, 291-297.	1.0	30
24	Gas phase Boudouard reactions involving singletâ€“singlet and singletâ€“triplet CO vibrationally excited states: implications for the non-equilibrium vibrational kinetics of CO/CO2 plasmas. European Physical Journal D, 2017, 71, 1.	0.6	29
25	The Astrochemical Observatory: Molecules in the Laboratory and in the Cosmos. Journal of the Chinese Chemical Society, 2012, 59, 1045-1052.	0.8	27
26	Control of conformers combining cooling by supersonic expansion of seeded molecular beams with hexapole selection and alignment: experiment and theory on 2-butanol. Physical Chemistry Chemical Physics, 2014, 16, 9866.	1.3	27
27	Hexapole-Oriented Asymmetric-Top Molecules and Their Stereodirectional Photodissociation Dynamics. Journal of Physical Chemistry A, 2016, 120, 5389-5398.	1.1	27
28	Chirality in molecular collision dynamics. Journal of Physics Condensed Matter, 2018, 30, 063003.	0.7	26
29	Carbon Oxides in Gas Flows and Earth and Planetary Atmospheres: State-to-State Simulations of Energy Transfer and Dissociation Reactions. Lecture Notes in Computer Science, 2013, , 17-31.	1.0	26
30	Potential Energy Surface for the H₂Oâ‹¯H₂ System. Journal of Physical Chemistry A, 2009, 113, 15047-15054.	1.1	25
31	Few-body quantum and many-body classical hyperspherical approaches to reactions and to cluster dynamics. Theoretical Chemistry Accounts, 2007, 117, 709-721.	0.5	22
32	Rovibrationally Excited Molecules on the Verge of a Triple Breakdown: Molecular and Roaming Mechanisms in the Photodecomposition of Methyl Formate. Journal of Physical Chemistry A, 2016, 120, 5155-5162.	1.1	22
33	Potential energy surfaces for van der waals complexes of rare gases with H₂S and H₂S₂: Extension to xenon interactions and hyperspherical harmonics representation. International Journal of Quantum Chemistry, 2012, 112, 834-847.	1.0	21
34	EXPLORING A CHEMICAL ROUTE FOR THE FORMATION OF STABLE ANIONS OF POLYYNES [C_nH^{â‹¯} (nÂ=Â2, 4)] IN MOLECULAR CLOUDS. Astrophysical Journal, 2016, 830, 2.	1.6	21
35	Models of Aged Magnesiumâ€“Silicateâ€“Hydrate Cements Based on the Lizardite and Talc Crystals: A Periodic DFT-GIPAW Investigation. Journal of Physical Chemistry C, 2017, 121, 7319-7330.	1.5	21
36	Stereodirectional images of molecules oriented by a variable-voltage hexapolar field: Fragmentation channels of 2-bromobutane electronically excited at two photolysis wavelengths. Journal of Chemical Physics, 2017, 147, 013917.	1.2	20

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37	â€œTransitivityâ€• A Code for Computing Kinetic and Related Parameters in Chemical Transformations and Transport Phenomena. Molecules, 2019, 24, 3478.	1.7	18
38	Resveratrol Supported on Magnesium DiHydroxide (Resv@MDH) Represents an Oral Formulation of Resveratrol With Better Gastric Absorption and Bioavailability Respect to Pure Resveratrol. Frontiers in Nutrition, 2020, 7, 570047.	1.6	18
39	Interactions of Hydrogen Molecules with Halogen-Containing Diatomics from Ab Initio Calculations: Spherical-Harmonics Representation and Characterization of the Intermolecular Potentials. Journal of Physical Chemistry A, 2016, 120, 5315-5324.	1.1	14
40	Roaming signature in photodissociation of carbonyl compounds. International Reviews in Physical Chemistry, 2018, 37, 217-258.	0.9	14
41	Double photoionization of propylene oxide: A coincidence study of the ejection of a pair of valence-shell electrons. Journal of Chemical Physics, 2018, 148, 114302.	1.2	13
42	Screens for Displaying Chirality Changing Mechanisms of a Series of Peroxides and Persulfides from Conformational Structures Computed by Quantum Chemistry. Lecture Notes in Computer Science, 2017, , 354-368.	1.0	13
43	The Astrochemical Observatory: Experimental and Computational Focus on the Chiral Molecule Propylene Oxide as a Case Study. Lecture Notes in Computer Science, 2017, , 267-280.	1.0	12
44	The spherical-harmonics representation for the interaction between diatomic molecules: The general case and applications to CO CO and CO HF. Journal of Molecular Spectroscopy, 2017, 337, 163-177.	0.4	11
45	Vectorial imaging of the photodissociation of 2-bromobutane oriented via hexapolar state selection. Physical Chemistry Chemical Physics, 2019, 21, 14164-14172.	1.3	11
46	Spherical and hyperspherical harmonics representation of van der Waals aggregates. AIP Conference Proceedings, 2016, , .	0.3	9
47	UV Photodissociation of Halothane in a Focused Molecular Beam: Space-Speed Slice Imaging of Competitive Bond Breaking into Spinâ€“Orbit-Selected Chlorine and Bromine Atoms. Journal of Physical Chemistry A, 2020, 124, 5288-5296.	1.1	9
48	Stereodynamic Imaging of Bromine Atomic Photofragments Eliminated from 1-Bromo-2-methylbutane Oriented via Hexapole State Selector. Journal of Physical Chemistry A, 2019, 123, 6635-6644.	1.1	8
49	Temperature dependence of rate constants for the H(D) + CH4 reaction in gas and aqueous phase: deformed Transition-State Theory study including quantum tunneling and diffusion effects. Structural Chemistry, 2020, 31, 609-617.	1.0	8
50	The astrochemical observatory: Computational and theoretical focus on molecular chirality changing torsions around O â€“ O and S â€“ S bonds. AIP Conference Proceedings, 2017, , .	0.3	7
51	Hyperspherical and related views of the dynamics of nanoclusters. Physica Scripta, 2009, 80, 048103.	1.2	6
52	Stereodirectional photodynamics: Experimental and theoretical perspectives. AIP Conference Proceedings, 2016, , .	0.3	6
53	Transient isomers in the photodissociation of bromoiodomethane. Journal of Chemical Physics, 2018, 148, 134307.	1.2	6
54	Effective Four-Center Model for the Photodissociation Dynamics of Methyl Formate. Lecture Notes in Computer Science, 2014, , 452-467.	1.0	6

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55	Rotational state-selection and alignment of chiral molecules by electrostatic hexapoles. AIP Conference Proceedings, 2016, , .	0.3	5
56	Nucleophilic substitution vs elimination reaction of bisulfide ions with substituted methanes: exploration of chiral selectivity by stereodirectional first-principles dynamics and transition state theory. Journal of Molecular Modeling, 2019, 25, 227.	0.8	5
57	Molecular Dynamics of Chiral Molecules in Hyperspherical Coordinates. Lecture Notes in Computer Science, 2019, , 413-427.	1.0	5
58	Quadrilaterals on the square screen of their diagonals: Regge symmetries of quantum mechanical spin networks and Grashof classical mechanisms of four-bar linkages. Rendiconti Lincei, 2019, 30, 67-81.	1.0	5
59	Hyperspherical coordinates and energy partitions for reactive processes and clusters. AIP Conference Proceedings, 2019, , .	0.3	5
60	Screen representation of structural properties of alanine in polypeptide chains. AIP Conference Proceedings, 2019, , .	0.3	5
61	Screens Displaying Structural Properties of Aminoacids in Polypeptide Chains: Alanine as a Case Study. Lecture Notes in Computer Science, 2019, , 439-449.	1.0	5
62	Stereodynamics: From elementary processes to macroscopic chemical reactions. AIP Conference Proceedings, 2015, , .	0.3	4
63	Photodissociation Dynamics of CO-Forming Channels on the Ground-State Surface of Methyl Formate at 248 nm: Direct Dynamics Study and Assessment of Generalized Multicenter Impulsive Models. Journal of Physical Chemistry A, 2021, 125, 1198-1220.	1.1	4
64	Potential Energy Surfaces for Water Interacting with Heteronuclear Diatomic Molecules: H2Oâ€“HF as a Case Study. Chemical Physics Letters, 2021, 776, 138692.	1.2	4
65	Molecular beam scattering experiments on noble gasâ€“propylene oxide: Total integral cross sections and potential energy surfaces of Heâ€“ and Neâ€“C3H6O. Journal of Chemical Physics, 2021, 155, 234301.	1.2	4
66	Potential Energy Surfaces for Noble Gas (Ar, Kr, Xe, Rn)â€“Propylene Oxide Systems: Analytical Formulation and Binding. Symmetry, 2022, 14, 249.	1.1	4
67	Screen mapping of structural and electric properties, chirality changing rates and racemization times of chiral peroxides and persulfides. AIP Conference Proceedings, 2018, , .	0.3	3
68	The astrochemical observatory: The interaction between helium and the chiral molecule propylene oxide. AIP Conference Proceedings, 2018, , .	0.3	3
69	Potential Energy Surface for the Interaction of Helium with the Chiral Molecule Propylene Oxide. Lecture Notes in Computer Science, 2018, , 593-604.	1.0	3
70	LY294002 Inhibits Intermediate Conductance Calcium-Activated Potassium (KCa3.1) Current in Human Glioblastoma Cells. Frontiers in Physiology, 2021, 12, 790922.	1.3	3
71	Chirality in molecular collisions. AIP Conference Proceedings, 2017, , .	0.3	2
72	Conformer Selection by Electrostatic Hexapoles: A Theoretical Study on 1-Chloroethanol and 2-Chloroethanol. Symmetry, 2022, 14, 317.	1.1	2

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73	Photodissociation of methyl formate: Conical intersections, roaming and triple fragmentation. AIP Conference Proceedings, 2015, , .	0.3	1
74	Acetone-Water Mixtures: Molecular Dynamics Using a Semiempirical Intermolecular Potential. Lecture Notes in Computer Science, 2017, , 3-13.	1.0	1
75	Angular distribution of bromine atomic photofragment in oriented 2-bromobutane via hexapole state selector. AIP Conference Proceedings, 2017, , .	0.3	1
76	Collisions of chiral molecules theoretical aspects and experiments. AIP Conference Proceedings, 2018, , .	0.3	1
77	Hypergeometric orthogonal polynomials as expansion basis sets for atomic and molecular orbitals: The Jacobi ladder. Advances in Quantum Chemistry, 2019, , 55-77.	0.4	1
78	The Increase of the Reactivity of Molecular Hydrogen with Hydroxyl Radical from the Gas Phase versus an Aqueous Environment: Quantum Chemistry and Transition State-Theory Calculations. Lecture Notes in Computer Science, 2019, , 450-459.	1.0	1
79	A Minimal Model of Potential Energy Surface for the CO2 â€“ CO System. Lecture Notes in Computer Science, 2021, , 351-362.	1.0	1
80	Photodissociation dynamics of CO-forming channel of methyl formate at 193â€‰nm: a computational study. Molecular Physics, 2022, 120, .	0.8	1
81	Desenvolvimento de SuperfÃcies de Energia Potencial para Sistemas de Cinco Corpos com CarÃ¡ter Quiral. Revista Processos QuÃmicos, 2008, 2, 37-50.	0.0	1
82	Hypergeometric Polynomials, Hyperharmonic Discrete and Continuous Expansions: Evaluations, Interconnections, Extensions. Lecture Notes in Computer Science, 2019, , 460-476.	1.0	0
83	Rate constants and first-principles trajectories for attack at tetrahedral carbon: Role of molecular orientation on chiral selectivity. AIP Conference Proceedings, 2019, , .	0.3	0
84	A Quantum Chemical Approach for the Characterization of the Interaction Potential of Propylene Oxide with Rare-Gas Atoms (He, Ne,ÂAr). Progress in Theoretical Chemistry and Physics, 2020, , 103-118.	0.2	0