Andrea Lombardi

List of Publications by Year
in descending order

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112 papers	2,325 citations	136885 32 h-index	265120 42 g-index
113 all docs	113 docs citations	113 times ranked	689 citing authors

#	Article	IF	Citations
1	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
2	A full dimensional grid empowered simulation of the CO₂ + CO₂ processes. Journal of Computational Chemistry, 2012, 33, 1806-1819.	1.5	69
3	Atomic and molecular data for spacecraft re-entry plasmas. Plasma Sources Science and Technology, 2016, 25, 033004.	1.3	69
4	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
5	Global view of classical clusters: the hyperspherical approach to structure and dynamics. Physical Chemistry Chemical Physics, 2002, 4, 5040-5051.	1.3	56
6	Simulation of oriented collision dynamics of simple chiral molecules. International Journal of Quantum Chemistry, 2011, 111, 1651-1658.	1.0	55
7	Energy transfer upon collision of selectively excited CO2 molecules: State-to-state cross sections and probabilities for modeling of atmospheres and gaseous flows. Journal of Chemical Physics, 2015, 143, 034307.	1.2	51
8	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
9	Spherical and hyperspherical representation of potential energy surfaces for intermolecular interactions. International Journal of Quantum Chemistry, 2011, 111, 318-332.	1.0	48
10	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
11	Advances in non-equilibrium $$\hbox {CO}_2$$ plasma kinetics: a theoretical and experimental review. European Physical Journal D, 2021, 75, 1.	0.6	47
12	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
13	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
14	Aligned molecular collisions and a stereodynamical mechanism for selective chirality. Rendiconti Lincei, 2011, 22, 125-135.	1.0	44
15	A highâ€level ab initio study of the N₂ + N₂ reaction channel. Journal of Computational Chemistry, 2013, 34, 2668-2676.	1.5	44
16	Phase-space invariants for aggregates of particles:â€ƒHyperangular momenta and partitions of the classical kinetic energy. Journal of Chemical Physics, 2004, 121, 5579-5589.	1.2	43
17	The origin of chiral discrimination: supersonic molecular beam experiments and molecular dynamics simulations of collisional mechanisms. Physica Scripta, 2008, 78, 058119.	1.2	43
18	Aligned molecules: chirality discrimination in photodissociation and in molecular dynamics. Rendiconti Lincei, 2013, 24, 299-308.	1.0	43

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19	Modeling of Energy Transfer From Vibrationally Excited CO₂ Molecules: Cross Sections and Probabilities for Kinetic Modeling of Atmospheres, Flows, and Plasmas. Journal of Physical Chemistry A, 2013, 117, 11430-11440.	1.1	43
20	Accurate analytic intermolecular potential for the simulation of Na+ and K+ ion hydration in liquid water. Journal of Molecular Liquids, 2015, 204, 192-197.	2.3	42
21	Collective hyperspherical coordinates for polyatomic molecules and clusters. Molecular Physics, 2000, 98, 1763-1770.	0.8	41
22	Isomerization dynamics and thermodynamics of ionic argon clusters. Journal of Chemical Physics, 2006, 125, 114307.	1.2	40
23	A comparison of interatomic potentials for rare gas nanoaggregates. Computational and Theoretical Chemistry, 2008, 852, 22-29.	1.5	40
24	Hyperspherical harmonics for polyatomic systems: Basis set for kinematic rotations. International Journal of Quantum Chemistry, 2002, 89, 277-291.	1.0	39
25	Hyperspherical harmonics for polyatomic systems: basis set for collective motions. Theoretical Chemistry Accounts, 2004, 111, 400-406.	0.5	39
26	Alignment and Chirality in Gaseous Flows. Journal of the Vacuum Society of Japan, 2010, 53, 645-653.	0.3	38
27	Hyperspherical representation of potential energy surfaces: intermolecular interactions in tetra-atomic and penta-atomic systems. Physica Scripta, 2011, 84, 028111.	1.2	38
28	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
29	Energy transfer dynamics and kinetics of elementary processes (promoted) by gasâ€phase CO₂â€N₂ collisions: Selectivity control by the anisotropy of the interaction. Journal of Computational Chemistry, 2016, 37, 1463-1475.	1.5	36
30	Hyperangular momenta and energy partitions in multidimensional many-particle classical mechanics: The invariance approach to cluster dynamics. Physical Review A, 2005, 72, .	1.0	35
31	A Bond-Bond Portable Approach to Intermolecular Interactions: Simulations for N-methylacetamide and Carbon Dioxide Dimers. Lecture Notes in Computer Science, 2012, , 387-400.	1.0	34
32	Modeling the Intermolecular Interactions and Characterization of the Dynamics of Collisional Autoionization Processes. Lecture Notes in Computer Science, 2013, , 69-83.	1.0	33
33	An innovative synergistic grid approach to the computational study of protein aggregation mechanisms. Journal of Molecular Modeling, 2014, 20, 2226.	0.8	32
34	Nanostructure Selectivity for Molecular Adsorption and Separation: the Case of Graphyne Layers. Journal of Physical Chemistry C, 2018, 122, 16195-16208.	1.5	32
35	Phase-Space Invariants as Indicators of the Critical Behavior of Nanoaggregates. Physical Review Letters, 2004, 93, 113402.	2.9	31
36	Normal and hyperspherical mode analysis of NO-doped Kr crystals upon Rydberg excitation of the impurity. Journal of Chemical Physics, 2007, 126, 174701.	1.2	30

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37	Molecular alignment and chirality in gaseous streams and vortices. Rendiconti Lincei, 2013, 24, 291-297.	1.0	30
38	Invariant energy partitions in chemical reactions and cluster dynamics simulations. Computational Materials Science, 2006, 35, 187-191.	1.4	29
39	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
40	The Astrochemical Observatory: Molecules in the Laboratory and in the Cosmos. Journal of the Chinese Chemical Society, 2012, 59, 1045-1052.	0.8	27
41	Hexapole-Oriented Asymmetric-Top Molecules and Their Stereodirectional Photodissociation Dynamics. Journal of Physical Chemistry A, 2016, 120, 5389-5398.	1.1	27
42	Chirality in molecular collision dynamics. Journal of Physics Condensed Matter, 2018, 30, 063003.	0.7	26
43	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
44	Specific heats of clusters near a phase transition: Energy partitions among internal modes. Chemical Physics Letters, 2006, 430, 424-428.	1.2	25
45	Water (H2O) m or Benzene (C6H6) n Aggregates to Solvate the Kâ€‰+â€‰?. Lecture Notes in Computer Science, 2013, , 1-15.	1.0	23
46	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
47	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
48	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
49	A force field for acetone: the transition from small clusters to liquid phase investigated by molecular dynamics simulations. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	19
50	Orthogonal Coordinates and Hyperquantization Algorithm. The NH₃ and H₃O⁺ Umbrella Inversion Levels. Journal of Physical Chemistry A, 2009, 113, 15355-15365.	1.1	17
51	Two-dimensional diamine-linked covalent organic frameworks for CO₂/N₂ capture and separation: theoretical modeling and simulations. Physical Chemistry Chemical Physics, 2020, 22, 25918-25929.	1.3	16
52	The Molecular Stirrer Catalytic Effect in Methane Ice Formation. Lecture Notes in Computer Science, 2014, , 585-600.	1.0	16
53	Quantum chemical and dynamical approaches to intra and intermolecular kinetics: The C_nH_{2n}O (n = 1, 2, 3) molecules. International Journal of Quantum Chemistry, 2011, 111, 1784-1791.	1.0	15
54	Aqueous N-methylacetamide: New analytic potentials and a molecular dynamics study. Journal of Molecular Liquids, 2016, 224, 792-800.	2.3	15

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55	Full Dimensional Potential Energy Function and Calculation of State-Specific Properties of the CO+N2 Inelastic Processes Within an Open Molecular Science Cloud Perspective. Frontiers in Chemistry, 2019, 7, 309.	1.8	15
56	Molecular Physics of Elementary Processes Relevant to Hypersonics: Atom-Molecule, Molecule-Molecule and Atoms-Surface Processes. The Open Plasma Physics Journal, 2014, 7, 48-59.	0.7	15
57	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
58	Roaming signature in photodissociation of carbonyl compounds. International Reviews in Physical Chemistry, 2018, 37, 217-258.	0.9	14
59	Molecular Dynamics of CH4/N2 Mixtures on a Flexible Graphene Layer: Adsorption and Selectivity Case Study. Frontiers in Chemistry, 2019, 7, 386.	1.8	14
60	Molecular dynamics simulations and hyperspherical mode analysis of NO in Kr crystals with the use of ab initio potential energy surfaces for the Krâ€NO complex. International Journal of Quantum Chemistry, 2008, 108, 1821-1830.	1.0	13
61	Binary Classification of Proteins by a Machine Learning Approach. Lecture Notes in Computer Science, 2020, , 549-558.	1.0	13
62	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
63	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
64	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
65	Vectorial imaging of the photodissociation of 2-bromobutane oriented via hexapolar state selection. Physical Chemistry Chemical Physics, 2019, 21, 14164-14172.	1.3	11
66	Collective hyperspherical coordinates for polyatomic molecules and clusters. Molecular Physics, 2000, 98, 1763-1770.	0.8	11
67	Vibrational Energy Transfer in CO+N2 Collisions: A Database for Vâ€“V and Vâ€“T/R Quantum-Classical Rate Coefficients. Molecules, 2021, 26, 7152.	1.7	11
68	Design and implementation of a Grid application for direct calculations of reactive rates. Computational and Theoretical Chemistry, 2013, 1022, 103-107.	1.1	10
69	Spherical and hyperspherical harmonics representation of van der Waals aggregates. AIP Conference Proceedings, 2016, , .	0.3	9
70	Collisional Energy Exchange in CO $$_2$$ â€“N $$_2$$ Gaseous Mixtures. Lecture Notes in Computer Science, 2016, , 246-257.	1.0	9
71	Toward a Generalized HÃ¼ckel Rule: The Electronic Structure of Carbon Nanocones. Journal of Physical Chemistry A, 2021, 125, 9819-9825.	1.1	8
72	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

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73	A New Method for Binary Classification of Proteins with Machine Learning. Lecture Notes in Computer Science, 2021, , 388-397.	1.0	7
74	Hyperspherical and related views of the dynamics of nanoclusters. Physica Scripta, 2009, 80, 048103.	1.2	6
75	Stereodirectional photodynamics: Experimental and theoretical perspectives. AIP Conference Proceedings, 2016, , .	0.3	6
76	Effective Four-Center Model for the Photodissociation Dynamics of Methyl Formate. Lecture Notes in Computer Science, 2014, , 452-467.	1.0	6
77	Grid Calculation Tools for Massive Applications of Collision Dynamics Simulations: Carbon Dioxide Energy Transfer. Lecture Notes in Computer Science, 2014, , 627-639.	1.0	6
78	Ion-Water Cluster Molecular Dynamics Using a Semiempirical Intermolecular Potential. Lecture Notes in Computer Science, 2015, , 355-370.	1.0	5
79	Rotational state-selection and alignment of chiral molecules by electrostatic hexapoles. AIP Conference Proceedings, 2016, , .	0.3	5
80	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
81	Molecular Simulations of CO$$_{2}$$/N$$_{2}$$/H$$_{2}$$O Gaseous Mixture Separation in Graphtriyne Membrane. Lecture Notes in Computer Science, 2019, , 374-387.	1.0	5
82	Molecular Dynamics of Chiral Molecules in Hyperspherical Coordinates. Lecture Notes in Computer Science, 2019, , 413-427.	1.0	5
83	The Invariance Approach to Structure and Dynamics: Classical Hyperspherical Coordinates. Lecture Notes in Computer Science, 2019, , 428-438.	1.0	5
84	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
85	Hyperspherical coordinates and energy partitions for reactive processes and clusters. AIP Conference Proceedings, 2019, , .	0.3	5
86	Screen representation of structural properties of alanine in polypeptide chains. AIP Conference Proceedings, 2019, , .	0.3	5
87	Confinement of $$hbox {CO}_{2}$$ inside carbon nanotubes. European Physical Journal D, 2021, 75, 1.	0.6	5
88	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
89	Carbon Capture and Separation from CO2/N2/H2O Gaseous Mixtures in Bilayer Graphtriyne: A Molecular Dynamics Study. Lecture Notes in Computer Science, 2020, , 489-501.	1.0	4
90	Statistics of partitions of the kinetic energy of small nanoclusters. Russian Journal of Physical Chemistry B, 2008, 2, 947-963.	0.2	3

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91	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
92	The astrochemical observatory: The interaction between helium and the chiral molecule propylene oxide. AIP Conference Proceedings, 2018, , .	0.3	3
93	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
94	Chirality in molecular collisions. AIP Conference Proceedings, 2017, , .	0.3	2
95	Distributed Gaussian orbitals for molecular calculations: application to simple systems. Molecular Physics, 2020, 118, 1615646.	0.8	2
96	Symmetry and deformations of cluster and biomolecules by invariant shape coordinates. AIP Conference Proceedings, 2021, , .	0.3	2
97	Umbrella Inversion Processes. Disentanglement of the Vibration-rotation Problem and Eigenfunctions. , 2012, , .		1
98	Statistics of energy partitions for many-particle systems in arbitrary dimension. Regular and Chaotic Dynamics, 2014, 19, 318-347.	0.3	1
99	Photodissociation of methyl formate: Conical intersections, roaming and triple fragmentation. AIP Conference Proceedings, 2015, , .	0.3	1
100	A Theoretical Investigation of 1-Butanol Unimolecular Decomposition. Lecture Notes in Computer Science, 2015, , 384-393.	1.0	1
101	Acetone-Water Mixtures: Molecular Dynamics Using a Semiempirical Intermolecular Potential. Lecture Notes in Computer Science, 2017, , 3-13.	1.0	1
102	Angular distribution of bromine atomic photofragment in oriented 2-bromobutane via hexapole state selector. AIP Conference Proceedings, 2017, , .	0.3	1
103	Collisions of chiral molecules theoretical aspects and experiments. AIP Conference Proceedings, 2018, , .	0.3	1
104	A Minimal Model of Potential Energy Surface for the CO2 â€“ CO System. Lecture Notes in Computer Science, 2021, , 351-362.	1.0	1
105	Gas Adsorption on Graphtriyne Membrane: Impact of the Induction Interaction Term on the Computational Cost. Lecture Notes in Computer Science, 2020, , 513-525.	1.0	1
106	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
107	Publisher's Note: Phase-Space Invariants as Indicators of the Critical Behavior of Nanoaggregates [Phys. Rev. Lett.93, 113402 (2004)]. Physical Review Letters, 2004, 93, .	2.9	0
108	Hypergeometric Polynomials, Hyperharmonic Discrete and Continuous Expansions: Evaluations, Interconnections, Extensions. Lecture Notes in Computer Science, 2019, , 460-476.	1.0	0

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109	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
110	Intermolecular Forces for the Interaction of H$$_{2}$$Oâ€“Graphtriyne Membrane: Contribution of Induction Effects. Lecture Notes in Computer Science, 2021, , 426-438.	1.0	0
111	Deactivation dynamics of carbon dioxide in gas phase at thermal and moderately high temperature regimes. Chemical Physics Letters, 2021, 779, 138850.	1.2	0
112	The CH$$_2$$CH$$_2$$ + OH Gas Phase Reaction: Formaldehyde and Acetaldehyde Formation Routes. Lecture Notes in Computer Science, 2021, , 581-593.	1.0	0