Sergio Rampino

List of Publications by Year
in descending order

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57 papers	1,096 citations	394421 19 h-index	414414 32 g-index
60 all docs	60 docs citations	60 times ranked	946 citing authors

#	Article	IF	Citations
1	Application: donation and backdonation in coordination chemistry. , 2022, , 175-189.		0
2	Relativity and chemistry. , 2022, , 191-204.		0
3	Towards open molecular science. , 2022, , 241-248.		0
4	The potential-energy surface. , 2022, , 45-58.		0
5	The atom and the bond. , 2022, , 151-166.		0
6	Scientific computing. , 2022, , 207-219.		0
7	Towards complexity. , 2022, , 107-115.		0
8	From reaction dynamics to chemical kinetics. , 2022, , 87-93.		0
9	Application: C + CH+ a†' C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:msubsup><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow><mml:mrow><mml:mo linebreak="badbreak" linebreakstyle="after">+</mml:mo></mml:mrow></mml:msubsup></mml:math> + H: an astrochemical reaction. , 2022, , 95-106.		0
10	Stochastic Modelling of 13C NMR Spin Relaxation Experiments in Oligosaccharides. Molecules, 2021, 26, 2418.	3.8	1
11	Gas-Phase Formation and Isomerization Reactions of Cyanoacetaldehyde, a Prebiotic Molecule of Astrochemical Interest. ACS Earth and Space Chemistry, 2021, 5, 1071-1082.	2.7	10
12	Charge-Flow Profiles along Curvilinear Paths: A Flexible Scheme for the Analysis of Charge Displacement upon Intermolecular Interactions. Molecules, 2021, 26, 6409.	3.8	3
13	Chemical bonding in cuprous complexes with simple nitriles: octet rule and resonance concepts versus quantitative charge-redistribution analysis. Physical Chemistry Chemical Physics, 2020, 22, 20238-20247.	2.8	3
14	A General User-Friendly Tool for Kinetic Calculations of Multi-Step Reactions within the Virtual Multifrequency Spectrometer Project. Applied Sciences (Switzerland), 2020, 10, 1872.	2.5	8
15	Chemical promenades: Exploring potentialâ€energy surfaces with immersive virtual reality. Journal of Computational Chemistry, 2020, 41, 1310-1323.	3.3	21
16	The Chemical Bond and sâ€“d Hybridization in Coinage Metal(I) Cyanides. Inorganic Chemistry, 2019, 58, 11716-11729.	4.0	17
17	Machine Learning of Potential-Energy Surfaces Within a Bond-Order Sampling Scheme. Lecture Notes in Computer Science, 2019, , 388-400.	1.3	2
18	Virtual reality tools for advanced modeling. AIP Conference Proceedings, 2019, , .	0.4	7

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19	Potential-Energy Surfaces for Ring-Puckering Motions of Flexible Cyclic Molecules through Cremerâ€“Pople Coordinates: Computation, Analysis, and Fitting. Journal of Chemical Theory and Computation, 2019, 15, 4280-4294.	5.3	23
20	Ferrocenes with simple chiral substituents: an in-depth theoretical and experimental VCD and ECD study. Physical Chemistry Chemical Physics, 2019, 21, 9419-9432.	2.8	19
21	Exploiting coordination geometry to selectively predict the Ïƒ-donor and Ï€-acceptor abilities of ligands: a back-and-forth journey between electronic properties and spectroscopy. Chemical Communications, 2018, 54, 2397-2400.	4.1	24
22	Charge-Displacement Analysis via Natural Orbitals for Chemical Valence in the Four-Component Relativistic Framework. Journal of Chemical Theory and Computation, 2018, 14, 1286-1296.	5.3	22
23	Diving into chemical bonding: An immersive analysis of the electron charge rearrangement through virtual reality. Journal of Computational Chemistry, 2018, 39, 2607-2617.	3.3	30
24	Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnicogen Interactions. Angewandte Chemie, 2018, 130, 14049-14053.	2.0	7
25	Unveiling the Sulfurâ€“Sulfur Bridge: Accurate Structural and Energetic Characterization of a Homochalcogen Intermolecular Bond. Angewandte Chemie - International Edition, 2018, 57, 15822-15826.	13.8	49
26	Unveiling the Sulfurâ€“Sulfur Bridge: Accurate Structural and Energetic Characterization of a Homochalcogen Intermolecular Bond. Angewandte Chemie, 2018, 130, 16048-16052.	2.0	5
27	Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnicogen Interactions. Angewandte Chemie - International Edition, 2018, 57, 13853-13857.	13.8	60
28	On the relation between carbonyl stretching frequencies and the donor power of chelating diphosphines in nickel dicarbonyl complexes. Physical Chemistry Chemical Physics, 2017, 19, 9028-9038.	2.8	25
29	Automated Simulation of Gas-Phase Reactions on Distributed and Cloud Computing Infrastructures. Lecture Notes in Computer Science, 2017, , 60-73.	1.3	2
30	Hollow Gold Cages and Their Topological Relationship to Dual Fullerenes. Chemistry - A European Journal, 2016, 22, 8823-8834.	3.3	17
31	Hollow Gold Cages and Their Topological Relationship to Dual Fullerenes. Chemistry - A European Journal, 2016, 22, 8709-8709.	3.3	0
32	Thermal Rate Coefficients for the Astrochemical Process C + CH⁺ â†' C₂⁺ + H by Ring Polymer Molecular Dynamics. Journal of Physical Chemistry A, 2016, 120, 9887-9893.	2.5	18
33	Fundamentals: general discussion. Faraday Discussions, 2016, 195, 139-169.	3.2	2
34	On the temperature dependence of the rate coefficient of formation of C$_2^+$ from C + CH⁺. Monthly Notices of the Royal Astronomical Society, 2016, 460, 2368-2375.	4.4	20
35	A Dynamics Investigation of the C + CH⁺â†' C₂⁺ H Reaction on an ab Initio Bond-Order-Like Potential. Journal of Physical Chemistry A, 2016, 120, 5125-5135.	2.5	15
36	Configuration-Space Sampling in Potential Energy Surface Fitting: A Space-Reduced Bond-Order Grid Approach. Journal of Physical Chemistry A, 2016, 120, 4683-4692.	2.5	15

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37	How Ï€ back-donation quantitatively controls the CO stretching response in classical and non-classical metal carbonyl complexes. Chemical Science, 2016, 7, 1174-1184.	7.4	158
38	Thermal Fluctuations on FÃ¶rster Resonance Energy Transfer in Dyadic Solar Cell Sensitizers: A Combined Ab Initio Molecular Dynamics and TDDFT Investigation. Journal of Physical Chemistry C, 2015, 119, 16490-16499.	3.1	6
39	Charge-displacement analysis via natural orbitals for chemical valence: Charge transfer effects in coordination chemistry. Journal of Chemical Physics, 2015, 142, 084112.	3.0	69
40	Goldâ€“superheavy-element interaction in diatomics and cluster adducts: A combined four-component Dirac-Kohn-Sham/charge-displacement study. Journal of Chemical Physics, 2015, 143, 024307.	3.0	17
41	Code interoperability and standard data formats in quantum chemistry and quantum dynamics: The Q5/D5Cost data model. Journal of Computational Chemistry, 2014, 35, 611-621.	3.3	22
42	An ab Initio Benchmark and DFT Validation Study on Gold(I)-Catalyzed Hydroamination of Alkynes. Journal of Chemical Theory and Computation, 2014, 10, 1021-1034.	5.3	57
43	Full Parallel Implementation of an All-Electron Four-Component Diracâ€“Kohnâ€“Sham Program. Journal of Chemical Theory and Computation, 2014, 10, 3766-3776.	5.3	21
44	A Grid Empowered Virtual Versus Real Experiment for the Barrierless Li + FH â†' LiF + H Reaction. Lecture Notes in Computer Science, 2014, , 571-584.	1.3	9
45	Efficient Parallel All-Electron Four-Component Diracâ€“Kohnâ€“Sham Program Using a Distributed Matrix Approach II. Journal of Chemical Theory and Computation, 2013, 9, 5356-5364.	5.3	21
46	Bond order uniform grids for quantum reactive scattering. International Journal of Quantum Chemistry, 2012, 112, 1818-1828.	2.0	10
47	A priori modeling of chemical reactions on computational grid platforms: Workflows and data models. Chemical Physics, 2012, 398, 192-198.	1.9	26
48	An extension of the grid empowered molecular simulator to quantum reactive scattering. Journal of Computational Chemistry, 2012, 33, 708-714.	3.3	26
49	A study of the impact of long range interactions on the reactivity of N + N<SUB align=right>2 using the Grid Empowered Molecular Simulator GEMS. International Journal of Web and Grid Services, 2010, 6, 196.	0.5	11
50	COMPCHEM: Progress Towards GEMS a Grid Empowered Molecular Simulator and Beyond. Journal of Grid Computing, 2010, 8, 571-586.	3.9	63
51	GriF: A Grid framework for a Web Service approach to reactive scattering. Computer Physics Communications, 2010, 181, 1179-1185.	7.5	38
52	Microscopic branching processes: The O + O₂ reaction and its relaxed potential representations. International Journal of Quantum Chemistry, 2010, 110, 358-367.	2.0	21
53	Accurate Quantum Dynamics on Grid Platforms: Some Effects of Long Range Interactions on the Reactivity of N + N2. Lecture Notes in Computer Science, 2010, , 1-12.	1.3	6
54	The O + O2 reaction: quantum detailed probabilities and thermal rate coefficients. Theoretical Chemistry Accounts, 2009, 123, 249-256.	1.4	19

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55	A comparison of the quantum state-specific efficiency of N + N2 reaction computed on different potential energy surfaces. Physical Chemistry Chemical Physics, 2009, 11, 1752.	2.8	30
56	A Comparison of the Isotope Effect for the N + N2 Reaction Calculated on Two Potential Energy Surfaces. Lecture Notes in Computer Science, 2008, , 1081-1093.	1.3	11
57	Thermal rate coefficients in collinear versus bent transition state reactions: the N+N₂case study. Physica Scripta, 2008, 78, 058116.	2.5	25