Sergio Rampino

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1689377/publications.pdf

Version: 2024-02-01

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	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
2	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
3	COMPCHEM: Progress Towards GEMS a Grid Empowered Molecular Simulator and Beyond. Journal of Grid Computing, 2010, 8, 571-586.	3.9	63
4	Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnicogen Interactions. Angewandte Chemie - International Edition, 2018, 57, 13853-13857.	13.8	60
5	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
6	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
7	GriF: A Grid framework for a Web Service approach to reactive scattering. Computer Physics Communications, 2010, 181, 1179-1185.	7.5	38
8	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
9	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
10	A priori modeling of chemical reactions on computational grid platforms: Workflows and data models. Chemical Physics, 2012, 398, 192-198.	1.9	26
11	An extension of the grid empowered molecular simulator to quantum reactive scattering. Journal of Computational Chemistry, 2012, 33, 708-714.	3.3	26
12	Thermal rate coefficients in collinear versus bent transition state reactions: the N+N₂case study. Physica Scripta, 2008, 78, 058116.	2.5	25
13	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
14	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
15	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
16	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
17	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
18	Microscopic branching processes: The O + O₂ reaction and its relaxed potential representations. International Journal of Quantum Chemistry, 2010, 110, 358-367.	2.0	21

#	Article	IF	Citations
19	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
20	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
21	Chemical promenades: Exploring potentialâ€energy surfaces with immersive virtual reality. Journal of Computational Chemistry, 2020, 41, 1310-1323.	3.3	21
22	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
23	The O + O2 reaction: quantum detailed probabilities and thermal rate coefficients. Theoretical Chemistry Accounts, 2009, 123, 249-256.	1.4	19
24	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
25	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
26	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
27	Hollow Gold Cages and Their Topological Relationship to Dual Fullerenes. Chemistry - A European Journal, 2016, 22, 8823-8834.	3.3	17
28	The Chemical Bond and sâ€“d Hybridization in Coinage Metal(I) Cyanides. Inorganic Chemistry, 2019, 58, 11716-11729.	4.0	17
29	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
30	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
31	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
32	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
33	Bond order uniform grids for quantum reactive scattering. International Journal of Quantum Chemistry, 2012, 112, 1818-1828.	2.0	10
34	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
35	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
36	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

#	Article	IF	Citations
37	Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnicogen Interactions. Angewandte Chemie, 2018, 130, 14049-14053.	2.0	7
38	Virtual reality tools for advanced modeling. AIP Conference Proceedings, 2019, , .	0.4	7
39	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
40	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
41	Unveiling the Sulfurâ€“Sulfur Bridge: Accurate Structural and Energetic Characterization of a Homochalcogen Intermolecular Bond. Angewandte Chemie, 2018, 130, 16048-16052.	2.0	5
42	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
43	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
44	Fundamentals: general discussion. Faraday Discussions, 2016, 195, 139-169.	3.2	2
45	Machine Learning of Potential-Energy Surfaces Within a Bond-Order Sampling Scheme. Lecture Notes in Computer Science, 2019, , 388-400.	1.3	2
46	Automated Simulation of Gas-Phase Reactions on Distributed and Cloud Computing Infrastructures. Lecture Notes in Computer Science, 2017, , 60-73.	1.3	2
47	Stochastic Modelling of 13C NMR Spin Relaxation Experiments in Oligosaccharides. Molecules, 2021, 26, 2418.	3.8	1
48	Hollow Gold Cages and Their Topological Relationship to Dual Fullerenes. Chemistry - A European Journal, 2016, 22, 8709-8709.	3.3	0
49	Application: donation and backdonation in coordination chemistry. , 2022, , 175-189.		0
50	Relativity and chemistry. , 2022, , 191-204.		0
51	Towards open molecular science. , 2022, , 241-248.		0
52	The potential-energy surface. , 2022, , 45-58.		0
53	The atom and the bond. , 2022, , 151-166.		0
54	Scientific computing. , 2022, , 207-219.		0

#	Article	IF	Citations
55	Towards complexity. , 2022, , 107-115.		0
56	From reaction dynamics to chemical kinetics. , 2022, , 87-93.		0
57	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