

Nicola Tasinato

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/8021647/publications.pdf>

Version: 2024-02-01

69
papers

1,577
citations

279798

23
h-index

361022

35
g-index

71
all docs

71
docs citations

71
times ranked

780
citing authors

#	ARTICLE	IF	CITATIONS
1	Accuracy and Interpretability: The Devil and the Holy Grail. New Routes across Old Boundaries in Computational Spectroscopy. <i>Chemical Reviews</i> , 2019, 119, 8131-8191.	47.7	167
2	Anharmonic theoretical simulations of infrared spectra of halogenated organic compounds. <i>Journal of Chemical Physics</i> , 2013, 139, 074310.	3.0	72
3	Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnictogen Interactions. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 13853-13857.	13.8	60
4	Development and Implementation of Advanced Fitting Methods for the Calculation of Accurate Molecular Structures. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3060-3075.	5.3	50
5	Accuracy Meets Interpretability for Computational Spectroscopy by Means of Hybrid and Double-Hybrid Functionals. <i>Frontiers in Chemistry</i> , 2020, 8, 584203.	3.6	50
6	Unveiling the Sulfur-Sulfur Bridge: Accurate Structural and Energetic Characterization of a Homochalcogen Intermolecular Bond. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 15822-15826.	13.8	49
7	Accurate Biomolecular Structures by the Nano-LEGO Approach: Pick the Bricks and Build Your Geometry. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7290-7311.	5.3	45
8	Structural features of the carbon-sulfur chemical bond: a semi-experimental perspective. <i>Canadian Journal of Chemistry</i> , 2016, 94, 1065-1076.	1.1	40
9	Noncovalent Interactions and Internal Dynamics in Pyridine-Ammonia: A Combined Quantum-Chemical and Microwave Spectroscopy Study. <i>Chemistry - A European Journal</i> , 2017, 23, 4876-4883.	3.3	39
10	Anharmonic force field and vibrational dynamics of CH ₂ F ₂ up to 5000 cm ⁻¹ studied by Fourier transform infrared spectroscopy and state-of-the-art <i>ab initio</i> calculations. <i>Journal of Chemical Physics</i> , 2012, 136, 214302.	3.0	37
11	An integrated experimental and quantum-chemical investigation on the vibrational spectra of chlorofluoromethane. <i>Journal of Chemical Physics</i> , 2013, 139, 164302.	3.0	36
12	Unveiling the non-covalent interactions of molecular homodimers by dispersion-corrected DFT calculations and collision-induced broadening of ro-vibrational transitions: application to (CH ₂ F) ₂ and (SO ₂) ₂ . <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 5659-5669.	2.8	36
13	Rotational and Infrared Spectroscopy of Ethanamine: A Route toward Its Astrophysical and Planetary Detection. <i>Astrophysical Journal</i> , 2018, 855, 123.	4.5	35
14	VMS-ROT: A New Module of the Virtual Multifrequency Spectrometer for Simulation, Interpretation, and Fitting of Rotational Spectra. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4382-4396.	5.3	34
15	Development and Validation of a Parameter-Free Model Chemistry for the Computation of Reliable Reaction Rates. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4913-4928.	5.3	34
16	Adsorption of F ₂ CCFCl on TiO ₂ nano-powder: Structures, energetics and vibrational properties from DRIFT spectroscopy and periodic quantum chemical calculations. <i>Applied Surface Science</i> , 2015, 353, 986-994.	6.1	28
17	Infrared Spectra, Integrated Band Intensities, and Anharmonic Force Field of H ₂ C=CHF. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1497-1504.	2.5	26
18	Spectroscopic measurements of SO ₂ line parameters in the 9.2-10.4 μm atmospheric region and theoretical determination of self-broadening coefficients. <i>Journal of Chemical Physics</i> , 2010, 132, 044315.	3.0	26

#	ARTICLE	IF	CITATIONS
19	On the competition between weak O H \cdots F and C H \cdots F hydrogen bonds, in cooperation with C H \cdots O contacts, in the difluoromethane \cdots tert-butyl alcohol cluster. <i>Journal of Molecular Spectroscopy</i> , 2017, 337, 90-95.	1.2	26
20	Microwave, High-Resolution Infrared, and Quantum Chemical Investigations of CHBrF ₂ : Ground and $v_4 = 1$ States. <i>Journal of Physical Chemistry A</i> , 2011, 115, 453-459.	2.5	25
21	Computing sextic centrifugal distortion constants by DFT: A benchmark analysis on halogenated compounds. <i>Journal of Molecular Spectroscopy</i> , 2017, 335, 117-125.	1.2	24
22	Correct Modeling of Cisplatin: a Paradigmatic Case. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 13838-13841.	13.8	24
23	A twist on the reaction of the CN radical with methylamine in the interstellar medium: new hints from a state-of-the-art quantum-chemical study. <i>Monthly Notices of the Royal Astronomical Society</i> , 2020, 496, 4298-4310.	4.4	24
24	DFT meets the segmented polarization consistent basis sets: Performances in the computation of molecular structures, rotational and vibrational spectroscopic properties. <i>Journal of Molecular Structure</i> , 2020, 1208, 127886.	3.6	23
25	Quantum cascade laser spectroscopy: diagnostics to non-linear optics. <i>Journal of Modern Optics</i> , 2009, 56, 2034-2048.	1.3	22
26	Quantum-chemical ab initio investigation of the vibrational spectrum of halon 1113 and its anharmonic force field: A joint experimental and computational approach. <i>Chemical Physics</i> , 2012, 397, 55-64.	1.9	22
27	Time dependent measurements of nitrous oxide and carbon dioxide collisional relaxation processes by a frequency down-chirped quantum cascade laser: Rapid passage signals and the time dependence of collisional processes. <i>Journal of Chemical Physics</i> , 2010, 132, 164301.	3.0	20
28	Toward a Complete Understanding of the Vinyl Fluoride Spectrum in the Atmospheric Region. <i>ChemPhysChem</i> , 2011, 12, 356-363.	2.1	20
29	N ₂ , O ₂ - and He-collision-induced broadening of sulfur dioxide ro-vibrational lines in the 9.2 μ m atmospheric window. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 118, 373-379.	3.9	20
30	The Role of State-of-the-Art Quantum-Chemical Calculations in Astrochemistry: Formation Route and Spectroscopy of Ethanamine as a Paradigmatic Case. <i>Molecules</i> , 2020, 25, 2873.	3.8	20
31	Spectroscopic study of CHBrF ₂ up to 9500 cm^{-1} : Vibrational analysis, integrated band intensities, and <i>ab initio</i> calculations. <i>Journal of Chemical Physics</i> , 2010, 133, 044310.	3.0	19
32	Accurate Vibrational \cdots Rotational Parameters and Infrared Intensities of 1-Bromo-1-fluoroethene: A Joint Experimental Analysis and Ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3305-3317.	2.5	18
33	CO ₂ , He- and H ₂ -broadening coefficients of SO ₂ for $\hat{\nu}_2$ band and ground state transitions for astrophysical applications. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2017, 203, 367-376.	2.3	18
34	Reinvestigation of the Deceptively Simple Reaction of Toluene with OH and the Fate of the Benzyl Radical: The \cdots Hidden \cdots Routes to Cresols and Benzaldehyde. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5917-5930.	2.5	18
35	Determination of the vinyl fluoride line intensities by TDL spectroscopy: the object oriented approach of Visual Line Shape Fitting Program to line profile analysis. <i>Molecular Physics</i> , 2010, 108, 677-685.	1.7	17
36	A complete listing of sulfur dioxide self-broadening coefficients for atmospheric applications by coupling infrared and microwave spectroscopy to semiclassical calculations. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2013, 130, 233-248.	2.3	17

#	ARTICLE	IF	CITATIONS
37	Study of the Vibrational Spectra and Absorption Cross Sections of 1-Chloro-1-fluoroethene by a Joint Experimental and Ab Initio Approach. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8369-8386.	2.5	17
38	State-of-the-art computation of the rotational and IR spectra of the methyl-cyclopropyl cation: hints on its detection in space. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 3431-3439.	2.8	17
39	An investigation of collisional processes in a Dicke narrowed transition of water vapor in the 7.8- $\hat{1}/4$ m spectral region by frequency down-chirped quantum cascade laser spectroscopy. <i>Journal of Chemical Physics</i> , 2010, 132, 044316.	3.0	16
40	Modelling the anharmonic and Coriolis resonances within the six level polyad involving the $\hat{1}/24$ fundamental in the ro-vibrational spectrum of vinyl fluoride. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2012, 113, 1240-1249.	2.3	16
41	What are the spectroscopic properties of HFC-32? Answers from DFT. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 1472-1485.	2.0	16
42	Towards the SMART workflow system for computational spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26034-26052.	2.8	16
43	Accurate Quantum Chemical Spectroscopic Characterization of Glycolic Acid: A Route Toward its Astrophysical Detection. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2373-2387.	2.5	16
44	Self-, N ₂ -, O ₂ -broadening coefficients and line parameters of HFC-32 for $\hat{1}/27$ band and ground state transitions from infrared and microwave spectroscopy. <i>Molecular Physics</i> , 2014, 112, 2384-2396.	1.7	15
45	Molecular synthons for accurate structural determinations: the equilibrium geometry of 1-chloro-1-fluoroethene. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 3615-3625.	2.8	15
46	The energetic of (CH ₂ F) ₂ investigated by TDL IR spectroscopy and DFT computations: From collision induced relaxation of ro-vibrational transitions to non-covalent interactions. <i>Journal of Chemical Physics</i> , 2015, 142, 134310.	3.0	14
47	FTIR spectra of CH ₂ F ₂ in the 1000-1300 cm ⁻¹ region: Rovibrational analysis and modeling of the Coriolis and anharmonic resonances in the $\hat{1}/23$, $\hat{1}/25$, $\hat{1}/27$, $\hat{1}/29$ and $2\hat{1}/24$ polyad. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2016, 175, 8-16.	2.3	14
48	Looking for the Elusive Imine Tautomer of Creatinine: Different States of Aggregation Studied by Quantum Chemistry and Molecular Spectroscopy. <i>ChemPlusChem</i> , 2021, 86, 1374-1386.	2.8	14
49	Exploring the Maze of C ₂ N ₂ H ₅ Radicals and Their Fragments in the Interstellar Medium with the Help of Quantum-Chemical Computations. <i>ACS Earth and Space Chemistry</i> , 2020, 4, 774-782.	2.7	13
50	High-Resolution Infrared Study of Vinyl Fluoride in the 750-1050 cm ⁻¹ Region: Rovibrational Analysis and Resonances Involving the $\hat{1}/28$, $\hat{1}/210$, and $\hat{1}/211$ Fundamentals. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13412-13418.	2.5	12
51	Anharmonic resonances in the CH chromophore overtone spectra of CHBrF ₂ . <i>Molecular Physics</i> , 2011, 109, 2163-2172.	1.7	12
52	Sextic centrifugal distortion constants: interplay of density functional and basis set for accurate yet feasible computations. <i>Molecular Physics</i> , 2020, 118, e1734678.	1.7	12
53	Isomerization and Fragmentation Reactions on the [C ₂ SH ₄] Potential Energy Surface: The Metastable Thione <i>S</i> -Methylide Isomer. <i>Journal of Organic Chemistry</i> , 2021, 86, 2941-2956.	3.2	11
54	Tailor-made computational protocols for precise characterization of small biological building blocks using QM and MM approaches. <i>Biopolymers</i> , 2018, 109, e23109.	2.4	10

#	ARTICLE	IF	CITATIONS
55	Modeling amino-acid side chain infrared spectra: the case of carboxylic residues. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 3008-3016.	2.8	10
56	Unraveling the role of additional OH-radicals in the H ₂ O abstraction from Dimethyl sulfide using quantum chemical computations. <i>Chemical Physics Letters</i> , 2020, 739, 136963.	2.6	9
57	The Spectroscopic Characterization of Halogenated Pollutants through the Interplay between Theory and Experiment: Application to R1122. <i>Molecules</i> , 2022, 27, 748.	3.8	8
58	Collisional Effects On Quantum Cascade Laser Induced Molecular Alignment. <i>AIP Conference Proceedings</i> , 2010, , .	0.4	7
59	A Bit of Sugar on TiO ₂ : Quantum Chemical Insights on the Interfacial Interaction of Glycolaldehyde over Titanium Dioxide. <i>Journal of Physical Chemistry C</i> , 2018, 122, 6041-6051.	3.1	7
60	Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnictogen Interactions. <i>Angewandte Chemie</i> , 2018, 130, 14049-14053.	2.0	7
61	Insights into the interaction between CH ₂ F ₂ and titanium dioxide: DRIFT spectroscopy and DFT analysis of the adsorption energetics. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 1614-1620.	3.9	6
62	Dipolar 1,3-dipolar cycloaddition of thioformaldehyde S-methylide (CH ₂ SCH ₃) ⁺ on SO ₂ . <i>Journal of Computational Chemistry</i> , 2022, 43, 1420-1433.	3.3	6
63	A Computational Journey across Nitroxide Radicals: From Structure to Spectroscopic Properties and Beyond. <i>Molecules</i> , 2021, 26, 7404.	3.8	5
64	Line-by-line spectroscopic parameters of HFC-32 ro-vibrational transitions within the atmospheric window around 8.2-11.4 μm. <i>Journal of Molecular Spectroscopy</i> , 2018, 348, 57-63.	1.2	4
65	Gliding on Ice in Search of Accurate and Cost-Effective Computational Methods for Astrochemistry on Grains: The Puzzling Case of the HCN Isomerization. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3111-3121.	5.3	4
66	Investigation of CHBrF ₂ adsorbed on TiO ₂ through IR spectroscopy and DFT calculations. <i>Vibrational Spectroscopy</i> , 2013, 65, 142-146.	2.2	3
67	Collision induced broadening of ν ₁ band and ground state spectral lines of sulfur dioxide perturbed by N ₂ and O ₂ . <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2017, 198, 155-163.	2.3	3
68	A computational insight into the relationship between side chain IR line shapes and local environment in fibril-like structures. <i>Journal of Chemical Physics</i> , 2021, 154, 084105.	3.0	1
69	Correct Modeling of Cisplatin: a Paradigmatic Case. <i>Angewandte Chemie</i> , 2017, 129, 14026-14029.	2.0	0