Cyril Falvo

List of Publications by Year
in descending order

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53	937	516710	477307
papers	citations	16 h-index	29 g-index

55	55	55	901
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Radiative relaxation in isolated large carbon clusters: Vibrational emission versus recurrent fluorescence. Journal of Chemical Physics, 2022, 156, 144305.	3.0	11
2	Extracting vibrational anharmonicities from short driven molecular dynamics trajectories. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	1
3	Infrared Spectroscopy of Chemically Diverse Carbon Clusters: A Data-Driven Approach. Journal of Physical Chemistry A, 2021, 125, 5509-5518.	2.5	6
4	Quantum modeling of the optical spectra of carbon cluster structural families and relation to the interstellar extinction UV bump. Astronomy and Astrophysics, 2020, 634, A62.	5.1	17
5	Mapping the structural diversity of C₆₀ carbon clusters and their infrared spectra. Astronomy and Astrophysics, 2019, 625, L11.	5.1	19
6	Simulating the structural diversity of carbon clusters across the planar-to-fullerene transition. Physical Review A, 2019, 99, .	2.5	16
7	Linear and non-linear infrared response of one-dimensional vibrational Holstein polarons in the anti-adiabatic limit: Optical and acoustical phonon models. Journal of Chemical Physics, 2018, 148, 074103.	3.0	0
8	Atomistic modeling of the infrared response of fullerenes under hydrostatic pressure. Journal of Physics Condensed Matter, 2018, 30, 474001.	1.8	1
9	Anharmonic vibrational spectroscopy of polycyclic aromatic hydrocarbons (PAHs). Journal of Chemical Physics, 2018, 149, 144102.	3.0	25
10	Isomerization kinetics of flexible molecules in the gas phase: Atomistic versus coarse-grained sampling. Journal of Chemical Physics, 2018, 149, 072334.	3.0	0
11	The excitonic qubit coupled with a phonon bath on a star graph: anomalous decoherence and coherence revivals. Quantum Information Processing, 2017, 16, 1.	2.2	5
12	Dehydrogenation effects on the stability of aromatic units in polycyclic aromatic hydrocarbons in the interstellar medium: A computational study at finite temperature. Molecular Astrophysics, 2017, 7, 9-18.	1.6	10
13	Valence shell threshold photoelectron spectroscopy of the CHxCN (x = 0-2) and CNC radicals. Journal of Chemical Physics, 2017, 147, 013908.	3.0	14
14	Exciton-phonon dynamics on complex networks: Comparison between a perturbative approach and exact calculations. Physical Review E, 2017, 96, 022304.	2.1	1
15	EXPERIMENTAL AND COMPUTATIONAL INVESTIGATIONS OF THE THRESHOLD PHOTOELECTRON SPECTRUM OF THE HCCN RADICAL. , 2017, , .		0
16	Synchrotron-based valence shell photoionization of CH radical. Journal of Chemical Physics, 2016, 144, 204307.	3.0	19
17	Mixed quantum-classical simulations of the vibrational relaxation of photolyzed carbon monoxide in a hemoprotein. Journal of Chemical Physics, 2016, 145, 054108.	3.0	2
18	A new interpretation of the meaning of the center of line slope from a two-dimensional infrared spectrum. Journal of Chemical Physics, 2016, 144, 234103.	3.0	4

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19	Vibrational-coherence measurement of nonequilibrium quantum systems by four-wave mixing. Physical Review A, 2015, 92, .	2.5	3
20	Ultrafast Dynamics of Carboxy-Hemoglobin: Two-Dimensional Infrared Spectroscopy Experiments and Simulations. Journal of Physical Chemistry Letters, 2015, 6, 2216-2222.	4.6	18
21	Photoionization spectroscopy of CH3C3N in the vacuum-ultraviolet range. Journal of Molecular Spectroscopy, 2015, 315, 206-216.	1.2	7
22	Photoionization of cold gas phase coronene and its clusters: Autoionization resonances in monomer, dimer, and trimer and electronic structure of monomer cation. Journal of Chemical Physics, 2014, 141, 164325.	3.0	27
23	Low-energy vibrational spectra of flexible diphenyl molecules: biphenyl, diphenylmethane, bibenzyl and 2-, 3- and 4-phenyltoluene. Physical Chemistry Chemical Physics, 2014, 16, 22062-22072.	2.8	14
24	Intramolecular Processes Revealed Using UV-Laser-Induced IR-Fluorescence: A New Perspective on the â€œChannel Threeâ€•of Benzene. Journal of Physical Chemistry Letters, 2014, 5, 1083-1090.	4.6	8
25	Atomistic Modeling of Vibrational Action Spectra in Polyatomic Molecules: Nuclear Quantum Effects. Journal of Physical Chemistry A, 2014, 118, 5427-5436.	2.5	11
26	STRUCTURE AND ELECTRONIC PROPERTIES OF IONIZED PAH CLUSTERS. , 2014, , .		0
27	VISIBLE PHOTODISSOCIATION SPECTRA OF THE 1-METHYL AND 2-METHYLNAPHTHALENE CATIONS: LASER SPECTROSCOPY AND THEORETICAL SIMULATIONS. , 2014, , .		0
28	Visible Photodissociation Spectra of the 1- and 2-Methylnaphthalene Cations: Laser Spectroscopy and Theoretical Simulations. Journal of Physical Chemistry A, 2013, 117, 13664-13672.	2.5	6
29	Lowest energy vibrational modes of some naphthalene derivatives: Azulene, quinoline, isoquinoline â€“ Experiment and theory. Chemical Physics Letters, 2013, 557, 53-58.	2.6	17
30	Effects of hydrogen dissociation on the infrared emission spectra of naphthalene: theoretical modeling. Physical Chemistry Chemical Physics, 2013, 15, 10241.	2.8	6
31	State-Selective Excitation of the CO Stretch in Carboxyhemoglobin by Mid-IR Laser Pulse Shaping: A Theoretical Investigation. Journal of Physical Chemistry A, 2013, 117, 12884-12888.	2.5	13
32	A simple but accurate potential for the naphthalene-argon complex: Applications to collisional energy transfer and matrix isolated IR spectroscopy. Journal of Chemical Physics, 2013, 138, 034305.	3.0	10
33	Vibrational ladder climbing in carboxy-hemoglobin: Effects of the protein environment. Journal of Chemical Physics, 2013, 138, 145101.	3.0	12
34	Probing the spin multiplicity of gas-phase polycyclic aromatic hydrocarbons through their infrared emission spectrum: A theoretical study. Journal of Chemical Physics, 2012, 137, 064303.	3.0	6
35	Two-Dimensional Double-Quantum Spectra Reveal Collective Resonances in an Atomic Vapor. Physical Review Letters, 2012, 108, 193201.	7.8	97
36	Infrared emission from photo-excited gaseous benzene: detection with a new home-made spectrometer. EAS Publications Series, 2012, 58, 379-384.	0.3	2

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37	Vibrational spectra of polyatomic molecules assisted by quantum thermal baths. Physical Chemistry Chemical Physics, 2012, 14, 10503.	2.8	29
38	Frequency Distribution of the Amide-I Vibration Sorted by Residues in Amyloid Fibrils Revealed by 2D-IR Measurements and Simulations. Journal of Physical Chemistry B, 2012, 116, 3322-3330.	2.6	31
39	Improving anharmonic infrared spectra using semiclassically prepared molecular dynamics simulations. Physical Chemistry Chemical Physics, 2012, 14, 2381.	2.8	27
40	A fluctuating quantum model of the CO vibration in carboxyhemoglobin. Journal of Chemical Physics, 2011, 134, 214106.	3.0	10
41	Simulation of Two Dimensional Ultraviolet (2DUV) Spectroscopy of Amyloid Fibrils. Nature Precedings, 2010, , .	0.1	0
42	Simulation of Two-Dimensional Ultraviolet Spectroscopy of Amyloid Fibrils. Journal of Physical Chemistry B, 2010, 114, 12150-12156.	2.6	20
43	Coherent infrared multidimensional spectra of the OH stretching band in liquid water simulated by direct nonlinear exciton propagation. Journal of Chemical Physics, 2009, 130, 184501.	3.0	49
44	2D-IR Experiments and Simulations of the Coupling between Amide-I and Ionizable Side Chains in Proteins: Application to the Villin Headpiece. Journal of Physical Chemistry B, 2009, 113, 11260-11273.	2.6	72
45	Coherent Two Dimensional Infrared Spectroscopy of a Cyclic Decapeptide Antamanide. A Simulation Study of the Amide-I and A Bands. Journal of Physical Chemistry B, 2008, 112, 12479-12490.	2.6	18
46	Fast energy transfer mediated by multi-quanta bound states in a nonlinear quantum lattice. Physica D: Nonlinear Phenomena, 2006, 221, 58-71.	2.8	10
47	Vibrational Self-Trapping in an Î±-Helix. Springer Series in Chemical Physics, 2005, , 401-403.	0.2	3
48	Vibron-polaron critical localization in a finite size molecular nanowire. Journal of Chemical Physics, 2005, 122, 014701.	3.0	15
49	Vibron-polaron in Î±-helices. II. Two-vibron bound states. Journal of Chemical Physics, 2005, 123, 184710.	3.0	39
50	Vibron-polaron in Î±-helices. I. Single-vibron states. Journal of Chemical Physics, 2005, 123, 184709.	3.0	41
51	Relaxation channels of two-vibron bound states in Î±-helix proteins. Physical Review E, 2004, 69, 041906.	2.1	36
52	Direct Observation of Self-Trapped Vibrational States inÎ±-Helices. Physical Review Letters, 2004, 93, 106405.	7.8	123
53	Energy fluctuations at the multicritical point in two-dimensional spin glasses. Journal of Physics A, 2002, 35, 8171-8178.	1.6	3