Adolfo Bastida

List of Publications by Year
in descending order

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97	1,555	257357	434063
papers	citations	24 h-index	31 g-index

104	104	104	1346
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Interlocked Supramolecular Polymers Created by Combination of Halogen- and Hydrogen-Bonding Interactions through Anion-Template Self-Assembly. Journal of the American Chemical Society, 2018, 140, 2041-2045.	6.6	55
2	A modified Ehrenfest method that achieves Boltzmann quantum state populations. Chemical Physics Letters, 2006, 417, 53-57.	1.2	44
3	A Theoretical Study of the Reaction of Î²-Carotene with the Nitrogen Dioxide Radical in Solution. Journal of Physical Chemistry B, 2010, 114, 4366-4372.	1.2	41
4	A theoretical study of the HgAr2(3P1â†1S0) vibronic spectrum. Journal of Chemical Physics, 1993, 98, 1007-1017.	1.2	40
5	The Ehrenfest method with quantum corrections to simulate the relaxation of molecules in solution: Equilibrium and dynamics. Journal of Chemical Physics, 2007, 126, 014503.	1.2	40
6	Si-BEARING MOLECULES TOWARD IRC+10216: ALMA UNVEILS THE MOLECULAR ENVELOPE OF CWLeo. Astrophysical Journal Letters, 2015, 805, L13.	3.0	40
7	Electron impact ionization of small argon clusters. Chemical Physics Letters, 1996, 249, 1-6.	1.2	38
8	Vibrational predissociation of the I2â‹¯Ne2 cluster: A molecular dynamics with quantum transitions study. Journal of Chemical Physics, 1998, 109, 6320-6328.	1.2	37
9	Optimal generalized internal vibrational coordinates and potential energy surface for the ground electronic state of SO2. Journal of Chemical Physics, 2001, 115, 139-148.	1.2	35
10	A Density Functional Theory Study of the Structure and Vibrational Spectra of Î²-Carotene, Capsanthin, and Capsorubin. Journal of Physical Chemistry A, 2008, 112, 4815-4825.	1.1	34
11	Instantaneous normal modes, resonances, and decay channels in the vibrational relaxation of the amide I mode of N-methylacetamide-D in liquid deuterated water. Journal of Chemical Physics, 2010, 132, 224501.	1.2	33
12	Optimization of vibrational coordinates. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 1681.	1.7	32
13	Competition between electronic and vibrational predissociation in Arâ€“I2(B): a molecular dynamics with quantum transitions study. Chemical Physics, 1999, 240, 229-239.	0.9	30
14	Molecular dynamics simulation of the I2(X)â‹¯Ar isomers population in a free-jet expansion: Thermodynamics versus kinetic control. Journal of Chemical Physics, 2002, 116, 1944-1953.	1.2	30
15	Antioxidant Properties of Î²-Carotene Isomers and Their Role in Photosystems: Insights from Ab Initio Simulations. Journal of Physical Chemistry A, 2012, 116, 3498-3506.	1.1	30
16	Intramolecular vibrational redistribution and fragmentation dynamics of I2â€Šâ‹¯â€ŠNen (n=2â€“6) clusters. Journal of Chemical Physics, 1999, 111, 239-244.	1.2	28
17	Simulation of the Ar3+ absorption spectrum using Molecular Dynamics. Chemical Physics, 1996, 209, 291-298.	0.9	27
18	Hybrid quantum/classical simulation and kinetic study of the vibrational predissociation of Cl2â‹¯Nen (n=2,â€Š3). Journal of Chemical Physics, 1999, 111, 4577-4588.	1.2	27

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19	Importance of Polarization and Charge Transfer Effects to Model the Infrared Spectra of Peptides in Solution. Journal of Chemical Theory and Computation, 2011, 7, 1840-1849.	2.3	27
20	Determination of highly excited rovibrational states for N2O using generalized internal coordinates. Journal of Chemical Physics, 1999, 110, 6339-6352.	1.2	26
21	Vibrational Energy Relaxation of the Amide I Mode of N-Methylacetamide in D₂O Studied through Bornâ€“Oppenheimer Molecular Dynamics. Journal of Physical Chemistry B, 2014, 118, 6186-6197.	1.2	26
22	Matrix elements for the modified Pï¿½schl?Teller potential. International Journal of Quantum Chemistry, 1996, 57, 43-51.	1.0	25
23	Application of trajectory surface hopping to vibrational predissociation. Chemical Physics Letters, 1997, 280, 185-188.	1.2	25
24	Time evolution of reactants, intermediates, and products in the vibrational predissociation of Br2â‹¯Ne: A theoretical study. Journal of Chemical Physics, 2000, 113, 10130-10142.	1.2	24
25	Variational Calculations of Rovibrational Energies for CO2. Journal of Molecular Spectroscopy, 2001, 205, 62-72.	0.4	24
26	Density Functional Theory Study of the Stability and Vibrational Spectra of the Î²-Carotene Isomers. Journal of Physical Chemistry A, 2009, 113, 9899-9907.	1.1	24
27	HINTS OF A ROTATING SPIRAL STRUCTURE IN THE INNERMOST REGIONS AROUND IRC +10216. Astrophysical Journal, 2016, 818, 192.	1.6	24
28	Determination of a Potential Energy Surface for CO2Using Generalized Internal Vibrational Coordinates. Journal of Molecular Spectroscopy, 1999, 195, 137-146.	0.4	23
29	Curvilinear Jacobi and Radau normal coordinates for linear triatomic molecules. Application to CO2. Chemical Physics, 1993, 175, 255-264.	0.9	21
30	Atomistic Molecular Dynamics Simulations of the Interactions of Oleic and 2-Hydroxyoleic Acids with Phosphatidylcholine Bilayers. Journal of Physical Chemistry B, 2011, 115, 11727-11738.	1.2	21
31	Conformational changes of Î²-carotene and zeaxanthin immersed in a model membrane through atomistic molecular dynamics simulations. Physical Chemistry Chemical Physics, 2013, 15, 6527.	1.3	21
32	Formation of self-assembled supramolecular polymers by anti-electrostatic anionâ€“anion and halogen bonding interactions. Chemical Communications, 2020, 56, 7084-7087.	2.2	21
33	Full quantum vibrational simulation of the relaxation of the cyanide ion in water using the Ehrenfest method with quantum corrections. Journal of Chemical Physics, 2008, 129, 154501.	1.2	20
34	Hybrid Quantum/Classical Simulations of the Vibrational Relaxation of the Amide I Mode of N-Methylacetamide in D₂O Solution. Journal of Physical Chemistry B, 2012, 116, 2969-2980.	1.2	20
35	Vibrational dynamics of polyatomic molecules in solution: assignment, time evolution and mixing of instantaneous normal modes. Theoretical Chemistry Accounts, 2011, 128, 769-782.	0.5	19
36	Simulation of the photodissociation of Ar $_3^+$. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1997, 39, 325-331.	1.0	18

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37	Self-consistent-field calculation of vibrational bound states for triatomic molecules using transformed Jacobi coordinates. The Journal of Physical Chemistry, 1991, 95, 2292-2297.	2.9	17
38	Excited vibrational states and potential energy function for OCS determined using generalized internal coordinates. Journal of Chemical Physics, 2000, 113, 5695-5704.	1.2	17
39	Surface hopping simulation of the vibrational relaxation of I2 in liquid xenon using the collective probabilities algorithm. Journal of Chemical Physics, 2004, 121, 10611-10622.	1.2	16
40	Molecular Dynamics Simulations and Instantaneous Normal-Mode Analysis of the Vibrational Relaxation of the Câ^'H Stretching Modes ofN-methylacetamide-din Liquid Deuterated Water. Journal of Physical Chemistry A, 2010, 114, 11450-11461.	1.1	16
41	A method for analyzing the vibrational energy flow in biomolecules in solution. Journal of Chemical Physics, 2011, 135, 204106.	1.2	16
42	Twoâ€¢center matrix elements for Kratzer oscillators. Journal of Chemical Physics, 1990, 93, 3408-3412.	1.2	15
43	On the use of optimal internal vibrational coordinates for symmetrical bent triatomic molecules. Journal of Chemical Physics, 2005, 122, 224319.	1.2	15
44	Hybrid quantum/classical simulation of the vibrational relaxation of the bend fundamental in liquid water. Journal of Chemical Physics, 2009, 131, 204505.	1.2	15
45	Selective fluorescence sensing of H2PO4â^'by the anion induced formation of self-assembled supramolecular polymers. Organic and Biomolecular Chemistry, 2020, 18, 3858-3866.	1.5	15
46	Variational calculation of vibrational energies of triatomic molecules usingSCFoptimized modes. International Journal of Quantum Chemistry, 1991, 40, 685-694.	1.0	14
47	Hyperspherical Kinematic Vibrational Coordinates for Linear Triatomic Molecules. The Journal of Physical Chemistry, 1995, 99, 11051-11060.	2.9	14
48	Hydration Effect on Amide I Infrared Bands in Water: An Interpretation Based on an Interaction Energy Decomposition Scheme. Journal of Physical Chemistry B, 2015, 119, 9056-9067.	1.2	14
49	Vibrational energy redistribution during donorâ€“acceptor electronic energy transfer: criteria to identify subsets of active normal modes. Physical Chemistry Chemical Physics, 2020, 22, 18454-18466.	1.3	14
50	Use of rotated Jacobi coordinates to calculate vibrational levels of hydrogen cyanide. The Journal of Physical Chemistry, 1992, 96, 9691-9696.	2.9	13
51	Generalized hyperspherical coordinates for molecular vibrations. The Journal of Physical Chemistry, 1993, 97, 5831-5835.	2.9	13
52	Global potential energy surfaces for the CO2 and CS2 molecules. Chemical Physics Letters, 1999, 313, 670-678.	1.2	13
53	A theoretical study of the vibrational spectrum of the CS2 molecule. Journal of Chemical Physics, 2002, 116, 7495-7508.	1.2	13
54	Theoretical Study of the Temperature Dependence of the Vibrational Relaxation of the H₂O Bend Fundamental in Liquid Water and the Subsequent Distortion of the Hydrogen Bond Network. Journal of Physical Chemistry B, 2014, 118, 9427-9437.	1.2	13

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55	Improved analytic potential models for bent AB2 molecules. Journal of Molecular Spectroscopy, 1989, 136, 185-196.	0.4	12
56	Rovibrational energies, partition functions and equilibrium fractionation of the CO2 isotopologues. Journal of Quantitative Spectroscopy and Radiative Transfer, 2014, 147, 233-251.	1.1	12
57	Variational calculations of vibrational states of N2O using hyperspherical normal coordinates. Journal of Chemical Physics, 1996, 105, 6099-6110.	1.2	11
58	Optimal internal coordinates, vibrational spectrum, and effective Hamiltonian for ozone. Journal of Chemical Physics, 2007, 126, 244305.	1.2	11
59	Vibrational levels of water by the self-consistent-field method using Radau coordinates. The Journal of Physical Chemistry, 1992, 96, 4341-4346.	2.9	10
60	Optimal generalized internal vibrational coordinates for symmetrical linear triatomic molecules. Chemical Physics Letters, 1998, 298, 36-42.	1.2	10
61	Size evolution of the vibrational predissociation process in Br2Â·Â·Â·Nen clusters: Simulation and kinetic study. Faraday Discussions, 2001, 118, 257-268.	1.6	9
62	Theoretical calculations of vibrational frequencies and rotational constants of the N2O isotopomers. Journal of Molecular Spectroscopy, 2003, 217, 43-58.	0.4	9
63	Collective probabilities algorithm for surface hopping calculations. Journal of Chemical Physics, 2003, 119, 6489-6499.	1.2	9
64	Molecular dynamics with quantum transitions study of the vibrational relaxation of the HOD bend fundamental in liquid D2O. Journal of Chemical Physics, 2012, 136, 234507.	1.2	9
65	Conformational Changes of Trialanine in Water Induced by Vibrational Relaxation of the Amide I Mode. Journal of Physical Chemistry B, 2016, 120, 348-357.	1.2	9
66	Experimental and theoretical study of the photofragmentation process: Ar3++hÎ½â†'Ar2++Ar. Journal of Chemical Physics, 2000, 113, 2175-2181.	1.2	8
67	Using the Screened Coulomb Potential To Illustrate the Variational Method. Journal of Chemical Education, 2012, 89, 1152-1158.	1.1	8
68	On the Role of Entropy in the Stabilization of Î±-Helices. Journal of Chemical Information and Modeling, 2020, 60, 6523-6531.	2.5	8
69	Photoinduced Dynamics with Constrained Vibrational Motion: FrozeNM Algorithm. Journal of Chemical Theory and Computation, 2020, 16, 7289-7298.	2.3	7
70	Vibrational self-consistent-field approximation for triatomic molecules using hyperspherical modes with application to H2O. International Journal of Quantum Chemistry, 1992, 42, 475-488.	1.0	6
71	Modeling the production and fragmentation of Ar+3 after threshold photon impact ionization of Ar3. Journal of Chemical Physics, 1996, 104, 6907-6908.	1.2	6
72	On the interaction of a beam of polar molecules with a static and a resonant RF field as a source of molecular interferences. European Physical Journal D, 2008, 49, 297-303.	0.6	6

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73	Instantaneous normal mode analysis of the vibrational relaxation of the amide I mode of alanine dipeptide in water. Journal of Chemical Physics, 2013, 138, 205102.	1.2	6
74	Quantum solution of coupled harmonic oscillator systems beyond normal coordinates. Journal of Mathematical Chemistry, 2017, 55, 1964-1984.	0.7	6
75	Hostâ€"guest complexesvs.supramolecular polymers in chalcogen bonding receptors: an experimental and theoretical study. Dalton Transactions, 2022, 51, 1325-1332.	1.6	6
76	Excited state dynamics in HgAr2: statistical analysis of vibrational state distribution. Faraday Discussions, 1994, 97, 131-142.	1.6	5
77	Relaxation pathways of the OD stretch fundamental of HOD in liquid H2O. Journal of Chemical Physics, 2016, 145, 244502.	1.2	5
78	HIGH-RESOLUTION ROTATIONAL SPECTRUM, DUNHAM COEFFICIENTS, AND POTENTIAL ENERGY FUNCTION OF NaCl. Astrophysical Journal, 2016, 825, 150.	1.6	5
79	On the vibronic spectrum of small mercury-argon clusters. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1995, 92, 384-396.	0.2	5
80	A vibrational Hamiltonian model for triatomic molecules based on the Kratzer and Poschl Teller potentials. International Journal of Quantum Chemistry, 1994, 52, 165-175.	1.0	4
81	An analytical perturbation treatment of the rotating Morse oscillator. Journal of Physics B: Atomic, Molecular and Optical Physics, 2008, 41, 105102.	0.6	4
82	A spectroscopic potential energy surface for FCN. Journal of Quantitative Spectroscopy and Radiative Transfer, 2012, 113, 1155-1169.	1.1	4
83	Energetic Self-Folding Mechanism in Î±-Helices. Journal of Physical Chemistry B, 2019, 123, 8186-8194.	1.2	4
84	Efficient parabolic evaluation of coupling terms in hybrid quantum/classical simulations. Chemical Physics, 2009, 358, 57-60.	0.9	3
85	Theoretical vibrational terms and rotational constants for the 15N substituted isotopologues of N2O calculated using normal hyperspherical coordinates. Journal of Quantitative Spectroscopy and Radiative Transfer, 2012, 113, 26-46.	1.1	3
86	Quantum treatment of HÃ©nonâ€"Heiles systems using oblique coordinates. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 025101.	0.6	3
87	Quantum solutions of identical linearly coupled harmonic oscillators using oblique coordinates. Journal of Physics B: Atomic, Molecular and Optical Physics, 2019, 52, 055101.	0.6	3
88	Quantum description of linearly coupled harmonic oscillator systems using oblique coordinates. Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 025101.	0.6	3
89	Ab Initio Partition Functions and Thermodynamic Quantities for the Molecular Hydrogen Isotopologues. Journal of Physical Chemistry A, 2021, 125, 9226-9241.	1.1	3
90	Perturbative virtualSCF CItreatment for energy levels of coupled oscillator systems. International Journal of Quantum Chemistry, 1989, 36, 49-60.	1.0	2

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91	The Rotating Morseâ€“Pekeris Oscillator Revisited. Journal of Chemical Education, 2008, 85, 1675.	1.1	2
92	Understanding the connection between conformational changes of peptides and equilibrium thermal fluctuations. Physical Chemistry Chemical Physics, 2017, 19, 3459-3463.	1.3	2
93	Intraresidual Correlated Motions in Peptide Chains. Journal of Chemical Information and Modeling, 2019, 59, 4524-4527.	2.5	2
94	Perturbed Morse expansion for triatomic molecules. Computational and Theoretical Chemistry, 1988, 166, 357-362.	1.5	1
95	Vibrational Bound States of the He2Ne+ Cation. Journal of Physical Chemistry A, 2009, 113, 14896-14903.	1.1	1
96	Mixed quantum classical steps: a DVR hopping method. PhysChemComm, 2000, 3, 29-35.	0.8	0
97	A rotating spiral structure in the innermost regions around IRC+10216. Journal of Physics: Conference Series, 2016, 728, 022005.	0.3	0