David Lauvergnat

List of Publications by Year
in descending order

53	1,592	279487	301761
papers	citations	23 h-index	39 g-index

53	53	53	1071
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Exact numerical computation of a kinetic energy operator in curvilinear coordinates. Journal of Chemical Physics, 2002, 116, 8560.	1.2	182
2	Full-dimensional (15-dimensional) quantum-dynamical simulation of the protonated water dimer. I. Hamiltonian setup and analysis of the ground vibrational state. Journal of Chemical Physics, 2007, 127, 184302.	1.2	145
3	Role of Conjugation in the Stabilities and Rotational Barriers of Formamide and Thioformamide. An ab Initio Valence-Bond Study. Journal of the American Chemical Society, 1997, 119, 9478-9482.	6.6	134
4	Full dimensional (15-dimensional) quantum-dynamical simulation of the protonated water-dimer III: Mixed Jacobi-valence parametrization and benchmark results for the zero point energy, vibrationally excited states, and infrared spectrum. Journal of Chemical Physics, 2009, 130, 234305.	1.2	93
5	Quantum dynamics with sparse grids: A combination of Smolyak scheme and cubature. Application to methanol in full dimensionality. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 18-25.	2.0	58
6	Automatic computer procedure for generating exact and analytical kinetic energy operators based on the polyspherical approach. Journal of Chemical Physics, 2012, 136, 034107.	1.2	56
7	A harmonic adiabatic approximation to calculate highly excited vibrational levels of â€œfloppy moleculesâ€• Journal of Chemical Physics, 2001, 114, 6592-6604.	1.2	44
8	Reactive scattering of highly vibrationally excited oxygen molecules: Ozone formation?. Journal of Chemical Physics, 1998, 108, 3566-3573.	1.2	42
9	Conformational Dynamics Guides Coherent Exciton Migration in Conjugated Polymer Materials: First-Principles Quantum Dynamical Study. Physical Review Letters, 2018, 120, 227401.	2.9	40
10	Torsional energy levels of nitric acid in reduced and full dimensionality with ElVibRot and Tnum. Physical Chemistry Chemical Physics, 2010, 12, 8405.	1.3	39
11	Symmetry-breaking and near-symmetry-breaking in three-electron-bonded radical cations. Journal of Chemical Physics, 2001, 115, 90-102.	1.2	37
12	A harmonic adiabatic approximation to calculate vibrational states of ammonia. Chemical Physics, 2004, 305, 105-113.	0.9	33
13	Quantum study of the internal rotation of methanol in full dimensionality (1+11D): a harmonic adiabatic approximation. Chemical Physics Letters, 2003, 373, 344-349.	1.2	31
14	Automatic computer procedure for generating exact and analytical kinetic energy operators based on the polyspherical approach: General formulation and removal of singularities. Journal of Chemical Physics, 2013, 139, 204107.	1.2	31
15	Dynamics of complex molecular systems with numerical kinetic energy operators in generalized coordinates. Chemical Physics, 2006, 326, 500-508.	0.9	29
16	Photoinduced nonadiabatic dynamics of ethene: Six-dimensional wave packet propagations using two different approximations of the kinetic energy operator. Chemical Physics, 2007, 338, 186-199.	0.9	29
17	Improving anharmonic infrared spectra using semiclassically prepared molecular dynamics simulations. Physical Chemistry Chemical Physics, 2012, 14, 2381.	1.3	27
18	A simple and efficient evolution operator for time-dependent Hamiltonians: the Taylor expansion. Journal of Chemical Physics, 2007, 126, 204103.	1.2	25

#	Article	IF	Citations
19	A generalised 17-state vibronic-coupling Hamiltonian model for ethylene. Journal of Chemical Physics, 2012, 137, 084304.	1.2	25
20	Rovibrational spectroscopy using a kinetic energy operator in Eckart frame and the multi-configuration time-dependent Hartree (MCTDH) approach. Journal of Chemical Physics, 2014, 141, 114101.	1.2	25
21	Intramolecular Charge Transfer in 4-Aminobenzonitrile Does Not Need the Twist and May Not Need the Bend. Journal of Physical Chemistry Letters, 2015, 6, 1316-1320.	2.1	25
22	Fast and slow excited-state intramolecular proton transfer in 3-hydroxychromone: a two-state story?. Physical Chemistry Chemical Physics, 2017, 19, 6579-6593.	1.3	25
23	H2, HD, and D2 in the small cage of structure II clathrate hydrate: Vibrational frequency shifts from fully coupled quantum six-dimensional calculations of the vibration-translation-rotation eigenstates. Journal of Chemical Physics, 2019, 150, 154303.	1.2	25
24	The non-linear tendencies in homonuclear X-X bonds (X = Li to F) and the lone-pair bond weakening effect. An ab initio theoretical analysis. Computational and Theoretical Chemistry, 1995, 338, 283-291.	1.5	23
25	Intramolecular stretching vibrational states and frequency shifts of (H2)2 confined inside the large cage of clathrate hydrate from an eight-dimensional quantum treatment using small basis sets. Journal of Chemical Physics, 2019, 151, 124311.	1.2	23
26	Quantum and Quantum-Classical Studies of the Photoisomerization of a Retinal Chromophore Model. Journal of Chemical Theory and Computation, 2020, 16, 6032-6048.	2.3	23
27	Rovibrational energy levels of the F^{â^'}(H₂O) and F^{â^'}(D₂O) complexes. Physical Chemistry Chemical Physics, 2016, 18, 17678-17690.	1.3	22
28	Numerical and exact kinetic energy operator using Eckart conditions with one or several reference geometries: Application to HONO. Journal of Chemical Physics, 2016, 144, 084116.	1.2	21
29	Effect of the overall rotation on the cisâ€"trans isomerization of HONO induced by an external field. Physical Chemistry Chemical Physics, 2012, 14, 3791.	1.3	20
30	Numerical on-the-fly implementation of the action of the kinetic energy operator on a vibrational wave function: application to methanol. Molecular Physics, 2018, 116, 3701-3709.	0.8	19
31	On the applicability of a wavefunction-free, energy-based procedure for generating first-order non-adiabatic couplings around conical intersections. Journal of Chemical Physics, 2017, 147, 114114.	1.2	18
32	Vertical transition energies vs. absorption maxima: Illustration with the UV absorption spectrum of ethylene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 52-58.	2.0	17
33	A generalised vibronic-coupling Hamiltonian model for benzopyran. Journal of Chemical Physics, 2014, 140, 044301.	1.2	17
34	Internal Conversion and Intersystem Crossing with the Exact Factorization. Journal of Chemical Theory and Computation, 2020, 16, 4833-4848.	2.3	17
35	The effect of the condensed-phase environment on the vibrational frequency shift of a hydrogen molecule inside clathrate hydrates. Journal of Chemical Physics, 2018, 148, 144304.	1.2	16
36	Full-dimensional vibrational calculations of five-atom molecules using a combination of Radau and Jacobi coordinates: Applications to methane and fluoromethane. Journal of Chemical Physics, 2016, 144, 204302.	1.2	15

#	Article	IF	Citations
37	Spin-Orbit Interactions in Ultrafast Molecular Processes. Physical Review Letters, 2020, 124, 033001.	2.9	15
38	Controlled full adderâ€“subtractor by vibrational computing. Physical Chemistry Chemical Physics, 2010, 12, 15628.	1.3	13
39	Monitoring the Birth of an Electronic Wavepacket in a Molecule with Attosecond Time-Resolved Photoelectron Spectroscopy. Journal of Physical Chemistry A, 2014, 118, 8773-8778.	1.1	13
40	Does cage quantum delocalisation influence the translationâ€“rotational bound states of molecular hydrogen in clathrate hydrate?. Faraday Discussions, 2018, 212, 533-546.	1.6	13
41	Ultrafast internal conversion in 4-aminobenzonitrile occurs sequentially along the seam. Chemical Physics, 2018, 509, 30-36.	0.9	12
42	A generalized vibronic-coupling Hamiltonian for molecules without symmetry: Application to the photoisomerization of benzopyran. Journal of Chemical Physics, 2019, 150, 124109.	1.2	11
43	Relaxation dynamics through a conical intersection: Quantum and quantumâ€“classical studies. Journal of Chemical Physics, 2021, 154, 034104.	1.2	10
44	A Full Dimensionality Approach to Evaluate the Nonlinear Optical Properties of Molecules with Large Amplitude Anharmonic Tunneling Motions. Journal of Chemical Theory and Computation, 2013, 9, 520-532.	2.3	9
45	Vibrational Coupled Cluster Computations in Polyspherical Coordinates with the Exact Analytical Kinetic Energy Operator. Journal of Chemical Theory and Computation, 2020, 16, 4505-4520.	2.3	8
46	First-principles description of intra-chain exciton migration in an oligo(para-phenylene) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 387 204119.	1.2	8
47	Valence bond curve-crossing model of the 1,2-hydrogen shift in HCN and isovalent systems. Chemical Physics Letters, 2001, 350, 345-350.	1.2	7
48	Describing the photo-isomerization of a retinal chromophore model with coupled and quantum trajectories. Journal of Chemical Physics, 2022, 156, 184104.	1.2	6
49	Smolyak Algorithm Adapted to a Systemâ€“Bath Separation: Application to an Encapsulated Molecule with Large-Amplitude Motions. Journal of Chemical Theory and Computation, 2022, 18, 4366-4372.	2.3	5
50	Quantum dynamics with curvilinear coordinates: models and kinetic energy operator. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2022, 380, 20200388.	1.6	4
51	Electronic Structure and Excited States of the Collision Reaction O(³P) + C₂H₄: A Multiconfigurational Perspective. Journal of Physical Chemistry A, 2021, 125, 6075-6088.	1.1	3
52	Orbital Control of the Thermal Dissociation of X2N-NX2 Molecules (X = NH2, SH) into Conjugated NX2 .pi.-Radicals. Journal of the American Chemical Society, 1995, 117, 2106-2107.	6.6	2
53	Smolyak representations with absorbing boundary conditions for reaction path Hamiltonian model of reactive scattering. Chemical Physics Letters, 2022, 787, 139241.	1.2	2