Oriol Vendrell

List of Publications by Year
in descending order

87	3,413	136740	143772
papers	citations	32 h-index	57 g-index

96	96	96	2851
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Multilayer multiconfiguration time-dependent Hartree method: Implementation and applications to a Henonâ€“Heiles Hamiltonian and to pyrazine. Journal of Chemical Physics, 2011, 134, 044135.	1.2	296
2	Ultrafast electron diffraction imaging of bond breaking in di-ionized acetylene. Science, 2016, 354, 308-312.	6.0	243
3	Full dimensional (15-dimensional) quantum-dynamical simulation of the protonated water dimer. II. Infrared spectrum and vibrational dynamics. Journal of Chemical Physics, 2007, 127, 184303.	1.2	207
4	Dynamics and Infrared Spectroscopy of the Protonated Water Dimer. Angewandte Chemie - International Edition, 2007, 46, 6918-6921.	7.2	171
5	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
6	Imaging electronic quantum motion with light. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 11636-11640.	3.3	140
7	Femtosecond response of polyatomic molecules to ultra-intense hard X-rays. Nature, 2017, 546, 129-132.	13.7	139
8	The multi-layer multi-configuration time-dependent Hartree method for bosons: Theory, implementation, and applications. Journal of Chemical Physics, 2013, 139, 134103.	1.2	112
9	Electronic decoherence following photoionization: Full quantum-dynamical treatment of the influence of nuclear motion. Physical Review A, 2017, 95, .	1.0	103
10	Full dimensional (15 dimensional) quantum-dynamical simulation of the protonated water-dimer IV: Isotope effects in the infrared spectra of D(D2O)2+, H(D2O)2+, and D(H2O)2+ isotopologues. Journal of Chemical Physics, 2009, 131, 034308.	1.2	95
11	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
12	Non-equilibrium quantum dynamics of ultra-cold atomic mixtures: the multi-layer multi-configuration time-dependent Hartree method for bosons. New Journal of Physics, 2013, 15, 063018.	1.2	89
13	Potential Energy Landscape of the Photoinduced Multiple Proton-Transfer Process in the Green Fluorescent Protein:Â Classical Molecular Dynamics and Multiconfigurational Electronic Structure Calculations. Journal of the American Chemical Society, 2006, 128, 3564-3574.	6.6	80
14	Coherent dynamics in cavity femtochemistry: Application of the multi-configuration time-dependent Hartree method. Chemical Physics, 2018, 509, 55-65.	0.9	75
15	Collective Jahn-Teller Interactions through Light-Matter Coupling in a Cavity. Physical Review Letters, 2018, 121, 253001.	2.9	75
16	Strong Isotope Effects in the Infrared Spectrum of the Zundel Cation. Angewandte Chemie - International Edition, 2009, 48, 352-355.	7.2	74
17	Operation of the Proton Wire in Green Fluorescent Protein. A Quantum Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 5500-5511.	1.2	63
18	Solvent-assisted catalysis in the enolization of acetaldehyde radical cation. Chemical Physics Letters, 2001, 334, 112-118.	1.2	52

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19	Modifying the Nonradiative Decay Dynamics through Conical Intersections via Collective Coupling to a Cavity Mode. Journal of Physical Chemistry A, 2019, 123, 8832-8844.	1.1	52
20	Control of Nuclear Dynamics through Conical Intersections and Electronic Coherences. Physical Review Letters, 2018, 120, 123001.	2.9	49
21	Coherent Electron Hole Dynamics Near a Conical Intersection. Physical Review Letters, 2014, 113, 113003.	2.9	46
22	A proton between two waters: insight from full-dimensional quantum-dynamics simulations of the [H2Oâ€“Hâ€“OH2]+ cluster. Physical Chemistry Chemical Physics, 2008, 10, 4692.	1.3	44
23	Dynamics from noisy data with extreme timing uncertainty. Nature, 2016, 532, 471-475.	13.7	44
24	A Potential Energy Function for Heterogeneous Proton-Wires. Ground and Photoactive States of the Proton-Wire in the Green Fluorescent Protein. Journal of Chemical Theory and Computation, 2008, 4, 1138-1150.	2.3	40
25	Full dimensional quantum-mechanical simulations for the vibronic dynamics of difluorobenzene radical cation isomers using the multilayer multiconfiguration time-dependent Hartree method. Journal of Chemical Physics, 2012, 137, 134302.	1.2	40
26	Dynamics and spectroscopy of molecular ensembles in a lossy microcavity. Journal of Chemical Physics, 2020, 153, 044108.	1.2	40
27	On the intramolecular proton transfer of 3-hydroxyflavone in the first singlet excited state: A theoretical study. Chemical Physics, 2006, 325, 243-250.	0.9	38
28	Ultrafast Dynamics of Photoionized Acetylene. Physical Review Letters, 2011, 107, 263002.	2.9	38
29	Generation of Highly Damaging H₂O⁺ Radicals by Inner Valence Shell Ionization of Water. ChemPhysChem, 2010, 11, 1006-1009.	1.0	36
30	Photoinduced proton transfer from the green fluorescent protein chromophore to a water molecule: analysis of the transfer coordinate. Chemical Physics Letters, 2004, 396, 202-207.	1.2	34
31	Suppression and Enhancement of Thermal Chemical Rates in a Cavity. Journal of Physical Chemistry Letters, 2022, 13, 4441-4446.	2.1	34
32	Multiconfiguration time-dependent Hartree impurity solver for nonequilibrium dynamical mean-field theory. Physical Review B, 2015, 91, .	1.1	33
33	Ultrafast isomerization in acetylene dication after carbon K-shell ionization. Nature Communications, 2017, 8, 453.	5.8	31
34	UV-Photochemistry of the Disulfide Bond: Evolution of Early Photoproducts from Picosecond X-ray Absorption Spectroscopy at the Sulfur K-Edge. Journal of the American Chemical Society, 2018, 140, 6554-6561.	6.6	30
35	Photoinduced Vibrations Drive Ultrafast Structural Distortion in Lead Halide Perovskite. Journal of the American Chemical Society, 2020, 142, 16569-16578.	6.6	30
36	Ultrafast Charge Transfer of a Valence Double Hole in Glycine Driven Exclusively by Nuclear Motion. Physical Review Letters, 2015, 115, 143002.	2.9	29

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37	Light-Induced Radical Formation and Isomerization of an Aromatic Thiol in Solution Followed by Time-Resolved X-ray Absorption Spectroscopy at the Sulfur K-Edge. Journal of the American Chemical Society, 2017, 139, 4797-4804.	6.6	26
38	Nuclear dynamics during the resonant Auger decay of water molecules. Journal of Chemical Physics, 2009, 130, 154307.	1.2	23
39	Molecular Dynamics of Excited State Intramolecular Proton Transfer:â€‰ 2-(2â€˜-Hydroxyphenyl)-4-methyloxazole in Gas Phase, Solution, and Protein Environments. Journal of Physical Chemistry B, 2004, 108, 6616-6623.	1.2	22
40	A combined nuclear dynamics and electronic study of the coupling between the internal rotation of the methyl group and the intramolecular proton transfer in 5-methyltropolone. Journal of Chemical Physics, 2002, 117, 7525-7533.	1.2	21
41	Proton conduction along a chain of water molecules. Development of a linear model and quantum dynamical investigations using the multiconfiguration time-dependent Hartree method. Journal of Chemical Physics, 2005, 122, 104505.	1.2	18
42	Suitable coordinates for quantum dynamics: Applications using the multiconfiguration time-dependent Hartree (MCTDH) algorithm. Computational and Theoretical Chemistry, 2012, 990, 75-89.	1.1	18
43	Ultrafast Energy Transfer to Liquid Water by Subâ€Picosecond Highâ€Intensity Terahertz Pulses: An Abâ€…Initio Molecular Dynamics Study. Angewandte Chemie - International Edition, 2013, 52, 13685-13687.	7.2	18
44	Core-level transient absorption spectroscopy as a probe of electron hole relaxation in photoionized H⁺(H₂O)_n. Faraday Discussions, 2014, 171, 457-470.	1.6	17
45	Exploring the Effects of Intramolecular Vibrational Energy Redistribution on the Operation of the Proton Wire in Green Fluorescent Protein. Journal of Physical Chemistry B, 2008, 112, 13443-13452.	1.2	16
46	Ultrafast hydrogen migration in acetylene cation driven by non-adiabatic effects. Journal of Chemical Physics, 2013, 138, 094311.	1.2	15
47	Ultrafast Energy Transfer from Solvent to Solute Induced by Subpicosecond Highly Intense THz Pulses. Journal of Physical Chemistry B, 2015, 119, 8080-8086.	1.2	14
48	Prospects of Using High-Intensity THz Pulses To Induce Ultrafast Temperature-Jumps in Liquid Water. Journal of Physical Chemistry A, 2018, 122, 5211-5222.	1.1	14
49	Evidence for interatomic Coulombic decay in Xe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>K</mml:mi></mml:math>-shell-vacancy decay of XeF<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review A, 2012, 86, .	1.0	13
50	Non-adiabatic quantum dynamics without potential energy surfaces based on second-quantized electrons: Application within the framework of the MCTDH method. Journal of Chemical Physics, 2020, 153, 154110.	1.2	13
51	Non-Born-Oppenheimer dynamics of the photoionized Zundel cation: A quantum wavepacket and surface-hopping study. Journal of Chemical Physics, 2013, 138, 094313.	1.2	12
52	Ultrafast imaging of spontaneous symmetry breaking in a photoionized molecular system. Nature Communications, 2021, 12, 4233.	5.8	12
53	Laser control over the ultrafast Coulomb explosion of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>N</mml:mi><mml:mn>2</mml:mn></mml:msub /><mml:mrow><mml:mn>2</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:msup></mml:mrow></mml:math> after Auger decay: A quantum-dynamics investigation. Physical Review A, 2017, 95, .	1.0	11
54	Electron-rotation coupling in diatomics under strong-field excitation. Physical Review A, 2020, 102, .	1.0	11

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55	Competition between collective and individual conical intersection dynamics in an optical cavity. New Journal of Physics, 2022, 24, 073022.	1.2	11
56	On the planarity of the tropolone molecule in the <mml:math altimg="si4.gif" display="inline" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/co	1.2	10
57	Weak-field few-femtosecond VUV photodissociation dynamics of water isotopologues. Physical Review A, 2017, 96, .	1.0	10
58	Challenges in XUV Photochemistry Simulations: A Case Study on Ultrafast Fragmentation Dynamics of the Benzene Radical Cation. Journal of Physical Chemistry A, 2018, 122, 1004-1010.	1.1	10
59	Quantum state tomography of molecules by ultrafast diffraction. Nature Communications, 2021, 12, 5441.	5.8	10
60	Many-photon excitation of organic molecules in a cavityâ€”Superradiance as a measure of coherence. Journal of Chemical Physics, 2020, 153, 244107.	1.2	9
61	Correlated Dynamics of the Motion of Proton-Hole Wave Packets in a Photoionized Water Cluster. Physical Review Letters, 2013, 110, 038302.	2.9	8
62	Ultrafast Transfer and Transient Entrapment of Photoexcited Mg Electron in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Mg</mml:mi><mml:mrow><mml:mo>@</mml:mo><mml:msub><mml:mrow><mml:mi mathvariant="normal">C</mml:mi></mml:mrow><mml:mrow><mml:mn>60</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:mrow></mml:mm Physical Review Letters, 2021, 126, 183002.	2.9	7
63	Photodissociation dynamics of the NH molecule under intense VUV pulses. Physical Review Research, 2020, 2, .	1.3	7
64	Sensitivity of core-level spectroscopy to electrostatic environments of nitrile groups: An ab initio study. Structural Dynamics, 2017, 4, 054102.	0.9	6
65	Ultraviolet Pumpâ€“Probe Photodissociation Spectroscopy of Electron-Rotation Coupling in Diatomics. Journal of Physical Chemistry Letters, 2021, 12, 5534-5539.	2.1	6
66	Generalized discrete truncated Wigner approximation for nonadiabatic quantum-classical dynamics. Journal of Chemical Physics, 2021, 155, 024111.	1.2	6
67	Dynamics of fluctuations in a quantum system. Physical Review A, 2014, 89, .	1.0	5
68	A bosonic perspective on the classical mapping of fermionic quantum dynamics. Journal of Chemical Physics, 2021, 155, 134110.	1.2	5
69	Fast hydrogen elimination from the [Ru(PH3)3(CO)(H)2] and [Ru(PH3)4(H)2] complexes in the first singlet excited states: A diabatic quantum dynamics study. Journal of Chemical Physics, 2004, 121, 6258-6267.	1.2	4
70	Interatomic Coulombic decay of a Li dimer in a coupled electron and nuclear dynamics approach. Physical Review A, 2020, 102, .	1.0	4
71	Dynamical Jahn-Teller effects on the generation of electronic ring currents by circularly polarized light. Physical Review Research, 2021, 3, .	1.3	4
72	On the generation of electronic ring currents under vibronic coupling effects. Journal of Chemical Physics, 2020, 153, 224308.	1.2	4

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73	Femtosecond x-ray absorption spectroscopy of pyrazine at the nitrogen K-edge: on the validity of the Lorentzian limit. Journal of Physics B: Atomic, Molecular and Optical Physics, 2021, 54, 244003.	0.6	4
74	Electron-rotation coupling in UV photodissociation of aligned diatomics. Physical Review Research, 2022, 4, .	1.3	4
75	Correlated proton-electron hole dynamics in protonated water clusters upon extreme ultraviolet photoionization. Structural Dynamics, 2016, 3, 043203.	0.9	3
76	Subpicosecond energy transfer from a highly intense THz pulse to water: A computational study based on the TIP4P/2005 rigid-water-molecule model. Physical Review E, 2016, 93, 032124.	0.8	3
77	Carrier-envelope-phase measurement of sub-cycle UV pulses using angular photofragment distributions. Communications Physics, 2022, 5, .	2.0	3
78	Time-resolved x-ray/optical pump-probe simulations on N2 molecules. Structural Dynamics, 2019, 6, 024101.	0.9	2
79	On the virial theorem for a particle in a box: Accounting for Cauchy's boundary condition. American Journal of Physics, 2020, 88, 1103-1108.	0.3	2
80	Chemical reaction dynamics I and electron dynamics in molecules: general discussion. Faraday Discussions, 2014, 171, 145-168.	1.6	1
81	Instrumentation and methods: general discussion. Faraday Discussions, 2014, 171, 505-523.	1.6	1
82	Distributed Memory Parallelization of the Multi-Configuration Time-Dependent Hartree Method. , 2010, , 147-163.		1
83	Vibrational Spectroscopy and Molecular Dynamics. Physical Chemistry in Action, 2014, , 117-145.	0.1	1
84	Dipole-induced processes in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mi mathvariant="normal">HeH</mml:mi><mml:mo>+</mml:mo></mml:msup></mml:math> produced by an excited Li(<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 297 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow	1.0	1
85	Physic Ab Initio Investigation of Nonlinear Mode Coupling in C₆₀. Journal of Physical Chemistry Letters, 2017, 8, 5543-5547.	2.1	0
86	Molecular ionization enhancement by charge rearrangement at high X-ray intensity. EPJ Web of Conferences, 2019, 205, 06009.	0.1	0
87	UV-photochemistry of the biologically relevant thiol group and the disulfide bond: Evolution of early photoproducts from picosecond X-ray absorption spectroscopy at the sulfur K-Edge. EPJ Web of Conferences, 2019, 205, 09006.	0.1	0