Rodolphe Vuilleumier

List of Publications by Year
in descending order

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164 papers	5,676 citations	57719 44 h-index	95218 68 g-index
177 all docs	177 docs citations	177 times ranked	5195 citing authors

#	Article	IF	Citations
1	Transport and spectroscopy of the hydrated proton: A molecular dynamics study. Journal of Chemical Physics, 1999, 111, 4251-4266.	1.2	261
2	Electronic Structure and Solvation of Copper and Silver Ions:Â A Theoretical Picture of a Model Aqueous Redox Reaction. Journal of the American Chemical Society, 2004, 126, 3928-3938.	6.6	196
3	An extended empirical valence bond model for describing proton transfer in H+(H2O)n clusters and liquid water. Chemical Physics Letters, 1998, 284, 71-77.	1.2	173
4	Quantum Dynamics of an Excess Proton in Water Using an Extended Empirical Valence-Bond Hamiltonian. Journal of Physical Chemistry B, 1998, 102, 4261-4264.	1.2	159
5	Infrared Spectroscopy ofN-Methylacetamide Revisited by ab Initio Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2005, 1, 772-789.	2.3	151
6	Van der Waals effects in ab initio water at ambient and supercritical conditions. Journal of Chemical Physics, 2011, 135, 154503.	1.2	138
7	Infrared spectroscopy in the gas and liquid phase from first principle molecular dynamics simulations: application to small peptides. Molecular Physics, 2007, 105, 2857-2878.	0.8	137
8	Water and ions in clays: Unraveling the interlayer/micropore exchange using molecular dynamics. Geochimica Et Cosmochimica Acta, 2007, 71, 5089-5101.	1.6	135
9	Visualizing Chemical Reactions in Solution by Picosecond X-Ray Diffraction. Physical Review Letters, 2004, 92, 125505.	2.9	123
10	Including many-body effects in models for ionic liquids. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	117
11	Sulfur radical species form gold deposits on Earth. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 13484-13489.	3.3	107
12	Extracting effective normal modes from equilibrium dynamics at finite temperature. Journal of Chemical Physics, 2006, 125, 144106.	1.2	104
13	Chemisorption of Hydroxide on 2D Materials from DFT Calculations: Graphene versus Hexagonal Boron Nitride. Journal of Physical Chemistry Letters, 2016, 7, 4695-4700.	2.1	92
14	Dipole Moment, Hydrogen Bonding and IR Spectrum of Confined Water. ChemPhysChem, 2006, 7, 2464-2467.	1.0	91
15	Molecular density functional theory of solvation: From polar solvents to water. Journal of Chemical Physics, 2011, 134, 194102.	1.2	86
16	Ab InitioMolecular Dynamics for Molecules with Variable Numbers of Electrons. Physical Review Letters, 2002, 88, 213002.	2.9	82
17	Electronic properties of hard and soft ions in solution: Aqueous Na+ and Ag+ compared. Journal of Chemical Physics, 2001, 115, 3454-3468.	1.2	79
18	Molecular Density Functional Theory of Water. Journal of Physical Chemistry Letters, 2013, 4, 619-624.	2.1	76

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19	Molecular dynamics of an excess proton in water using a non-additive valence bond force field. Journal of Molecular Structure, 1997, 436-437, 555-565.	1.8	74
20	Ab Initio Molecular Dynamics Study of a Highly Concentrated LiCl Aqueous Solution. Journal of Chemical Theory and Computation, 2008, 4, 1040-1048.	2.3	74
21	Water nanodroplets confined in zeolite pores. Faraday Discussions, 2009, 141, 377-398.	1.6	71
22	Molecular Hydrodynamics from Memory Kernels. Physical Review Letters, 2016, 116, 147804.	2.9	68
23	Nuclear velocity perturbation theory for vibrational circular dichroism: An approach based on the exact factorization of the electron-nuclear wave function. Journal of Chemical Physics, 2015, 143, 074106.	1.2	67
24	Versatile electrification of two-dimensional nanomaterials in water. Nature Communications, 2019, 10, 1656.	5.8	66
25	Improved modeling of liquid<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>GeSe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> Impact of the exchange-correlation functional. Physical Review B, 2009, 79, .	2.4	63
26	Ultrafast Nonadiabatic Fragmentation Dynamics of Doubly Charged Uracil in a Gas Phase. Physical Review Letters, 2011, 107, 023202.	2.9	63
27	Time-resolved x-ray diffraction: Statistical theory and its application to the photo-physics of molecular iodine. Journal of Chemical Physics, 2002, 116, 10615-10625.	1.2	61
28	Carbon dioxide transport in molten calcium carbonate occurs through an oxo-Grotthuss mechanism via a pyrocarbonate anion. Nature Chemistry, 2016, 8, 454-460.	6.6	60
29	Thermal versus electronic broadening in the density of states of liquid water. Chemical Physics Letters, 2003, 376, 68-74.	1.2	59
30	Recombination of photodissociated iodine: A time-resolved x-ray-diffraction study. Journal of Chemical Physics, 2006, 124, 034501.	1.2	59
31	Computer modeling of natural silicate melts: What can we learn from ab initio simulations. Geochimica Et Cosmochimica Acta, 2009, 73, 6313-6339.	1.6	58
32	A transferable ab initio based force field for aqueous ions. Journal of Chemical Physics, 2012, 136, 114507.	1.2	58
33	Structure, equation of state and transport properties of molten calcium carbonate (CaCO3) by atomistic simulations. Geochimica Et Cosmochimica Acta, 2014, 141, 547-566.	1.6	56
34	Equilibrium magnesium isotope fractionation between aqueous Mg2+ and carbonate minerals: Insights from path integral molecular dynamics. Geochimica Et Cosmochimica Acta, 2015, 163, 126-139.	1.6	55
35	Vibrational circular dichroism from ab initio molecular dynamics and nuclear velocity perturbation theory in the liquid phase. Journal of Chemical Physics, 2016, 145, 084101.	1.2	53
36	Direct observation of water-mediated single-proton transport between hBN surface defects. Nature Nanotechnology, 2020, 15, 598-604.	15.6	52

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37	A multi-scaleab initiotheoretical study of the production of free radicals in swift ion tracks in liquid water. Journal of Physics B: Atomic, Molecular and Optical Physics, 2007, 40, 1-12.	0.6	51
38	Chiral Crystal Packing Induces Enhancement of Vibrational Circular Dichroism. Angewandte Chemie - International Edition, 2018, 57, 13344-13348.	7.2	51
39	Investigation of structure and dynamics of the hydrated metalâ€“organic framework MIL-53(Cr) using first-principles molecular dynamics. Physical Chemistry Chemical Physics, 2013, 15, 19049.	1.3	50
40	Nuclear Velocity Perturbation Theory of Vibrational Circular Dichroism. Journal of Chemical Theory and Computation, 2013, 9, 5305-5312.	2.3	49
41	Hopping along hydrogen bonds. Nature Chemistry, 2012, 4, 432-433.	6.6	46
42	A topological analysis of the proton transfer in H5O2+. Molecular Physics, 1999, 96, 265-273.	0.8	46
43	The physics of liquid water. Comptes Rendus - Geoscience, 2005, 337, 159-171.	0.4	45
44	Timeâ€Dependent Density Functional Theory Molecular Dynamics Simulations of Liquid Water Radiolysis. ChemPhysChem, 2008, 9, 2099-2103.	1.0	45
45	Environmental effects on vibrational properties of carotenoids: experiments and calculations on peridinin. Physical Chemistry Chemical Physics, 2011, 13, 20954.	1.3	45
46	Ab Initio Simulation of Carbon Clustering on an Ni(111) Surface:Â A Model of the Poisoning of Nickel-Based Catalystsâ€. Journal of Physical Chemistry B, 2006, 110, 3638-3646.	1.2	44
47	Silver in geological fluids from in situ X-ray absorption spectroscopy and first-principles molecular dynamics. Geochimica Et Cosmochimica Acta, 2013, 106, 501-523.	1.6	44
48	Density functional calculation of the electronic absorption spectrum of Cu+ and Ag+ aqua ions. Journal of Chemical Physics, 2004, 121, 11885-11899.	1.2	43
49	Two algorithms to compute projected correlation functions in molecular dynamics simulations. Journal of Chemical Physics, 2014, 140, 124103.	1.2	43
50	Extension of Marcus Picture for Electron Transfer Reactions with Large Solvation Changes. Journal of the American Chemical Society, 2012, 134, 2067-2074.	6.6	42
51	Scalar fundamental measure theory for hard spheres in three dimensions: Application to hydrophobic solvation. Journal of Chemical Physics, 2012, 137, 034115.	1.2	42
52	An Extended Empirical Valence Bond Model for Describing Proton Mobility in Water. Israel Journal of Chemistry, 1999, 39, 457-467.	1.0	41
53	Polarizabilities of individual molecules and ions in liquids from first principles. Journal of Physics Condensed Matter, 2008, 20, 494207.	0.7	39
54	Computation of pair distribution functions and three-dimensional densities with a reduced variance principle. Molecular Physics, 2013, 111, 3486-3492.	0.8	39

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55	From Localized Orbitals to Material Properties: Building Classical Force Fields for Nonmetallic Condensed Matter Systems. Physical Review Letters, 2010, 104, 138301.	2.9	36
56	Density functional theory based molecular dynamics study of hydration and electronic properties of aqueous La3+. Journal of Chemical Physics, 2010, 133, 044509.	1.2	36
57	Ultrafast Damage Following Radiationâ€Induced Oxidation of Uracil in Aqueous Solution. Angewandte Chemie - International Edition, 2013, 52, 3160-3163.	7.2	34
58	Time-resolved observation of the Eigen cation in liquid water. Journal of Chemical Physics, 2007, 126, 034511.	1.2	33
59	Lanthanoids(III) and actinoids(III) in water: Diffusion coefficients and hydration enthalpies from polarizable molecular dynamics simulations. Pure and Applied Chemistry, 2012, 85, 237-246.	0.9	33
60	Computing Wigner distributions and time correlation functions using the quantum thermal bath method: application to proton transfer spectroscopy. Physical Chemistry Chemical Physics, 2013, 15, 12591.	1.3	32
61	A topological analysis of the proton transfer in H₅O⁺₂. Molecular Physics, 1999, 96, 265-273.	0.8	31
62	X-ray â€œfilmingâ€•of atomic motions in chemical reactions. Chemical Physics, 2004, 304, 245-251.	0.9	31
63	Theoretical investigation of the ultrafast dissociation of ionised biomolecules immersed in water: Direct and indirect effects. Mutation Research - Reviews in Mutation Research, 2010, 704, 45-53.	2.4	31
64	Insight into the Li2CO3â€“K2CO3 eutectic mixture from classical molecular dynamics: Thermodynamics, structure, and dynamics. Journal of Chemical Physics, 2016, 144, 104507.	1.2	31
65	Assessing cluster models of solvation for the description of vibrational circular dichroism spectra: synergy between static and dynamic approaches. Physical Chemistry Chemical Physics, 2020, 22, 26047-26068.	1.3	31
66	Carbon dioxide in silicate melts at upper mantle conditions: Insights from atomistic simulations. Chemical Geology, 2015, 418, 77-88.	1.4	29
67	The molecular structure of melts along the carbonatiteâ€“kimberliteâ€“basalt compositional joint: CO 2 and polymerisation. Earth and Planetary Science Letters, 2016, 434, 129-140.	1.8	29
68	Molecular Dynamics Simulations of a Silver Atom in Water: Evidence for a Dipolar Excitonic State. Physical Review Letters, 2003, 91, 208304.	2.9	28
69	Unravelling the Hydration Structure of ThX₄ (X = Br, Cl) Water Solutions by Molecular Dynamics Simulations and X-ray Absorption Spectroscopy. Journal of Physical Chemistry B, 2012, 116, 6465-6475.	1.2	28
70	Molecular Property Investigations of anortho-Hydroxy Schiff Base Type Compound with the First-Principle Molecular Dynamics Approach. Journal of Physical Chemistry B, 2010, 114, 242-253.	1.2	27
71	A NMR and molecular dynamics study of CO2-bearing basaltic melts and glasses. Chemical Geology, 2015, 418, 89-103.	1.4	27
72	On the Mass of Atoms in Molecules: Beyond the Born-Oppenheimer Approximation. Physical Review X, 2017, 7, .	2.8	26

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73	Mechanisms of the Waterâ^'Gas-Shift Reaction by Iron Pentacarbonyl in the Gas Phase. Inorganic Chemistry, 2008, 47, 8635-8640.	1.9	25
74	Challenges in first-principles NPT molecular dynamics of soft porous crystals: A case study on MIL-53(Ga). Journal of Chemical Physics, 2014, 141, 064703.	1.2	25
75	Equilibrium fractionation of H and O isotopes in water from path integral molecular dynamics. Geochimica Et Cosmochimica Acta, 2014, 135, 203-216.	1.6	25
76	Fermi Resonance as a Tool for Probing Peridinin Environment. Journal of Physical Chemistry B, 2014, 118, 5873-5881.	1.2	24
77	Fully Quantum Description of the Zundel Ion: Combining Variational Quantum Monte Carlo with Path Integral Langevin Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 2400-2417.	2.3	24
78	Effect of puckering motion and hydrogen bond formation on the vibrational circular dichroism spectrum of a flexible molecule: the case of (S)-1-indanol. Physical Chemistry Chemical Physics, 2018, 20, 14635-14646.	1.3	24
79	Molecular Dynamics Study of the Coordination Sphere of Trivalent Lanthanum in a Highly Concentrated LiCl Aqueous Solution: a Combined Classical and Ab Initio Approach. Journal of Physical Chemistry B, 2008, 112, 10603-10607.	1.2	23
80	Solvation of complex surfaces via molecular density functional theory. Journal of Chemical Physics, 2012, 137, 224107.	1.2	23
81	Hydrothermal Breakdown of Flexible Metalâ€“Organic Frameworks: A Study by First-Principles Molecular Dynamics. Journal of Physical Chemistry Letters, 2015, 6, 4365-4370.	2.1	23
82	Computation of Solid-State Vibrational Circular Dichroism in the Periodic Gauge. Journal of Physical Chemistry Letters, 2021, 12, 7213-7220.	2.1	23
83	Sparse matrix wave-front estimators for adaptive-optics systems for large ground-based telescopes. Optics Letters, 1995, 20, 955.	1.7	22
84	Ionization and fragmentation of water clusters by fast highly charged ions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2009, 42, 075101.	0.6	22
85	Stability and Instability of the Isoelectronic UO22+and PaO2+Actinyl Oxo-Cations in Aqueous Solution from Density Functional Theory Based Molecular Dynamics. Journal of Physical Chemistry B, 2011, 115, 3560-3570.	1.2	22
86	Modeling proton-induced damage on 2-deoxy-D-ribose. Conformational analysis. Journal of Molecular Modeling, 2014, 20, 2221.	0.8	22
87	Hydration properties of Cm(iii) and Th(iv) combining coordination free energy profiles with electronic structure analysis. Physical Chemistry Chemical Physics, 2014, 16, 5824.	1.3	21
88	Computation of electronic chemical potentials using free energy density functionals. Computational and Theoretical Chemistry, 2000, 506, 343-353.	1.5	19
89	Fermi resonance in CO2: Mode assignment and quantum nuclear effects from first principles molecular dynamics. Journal of Chemical Physics, 2017, 146, 134102.	1.2	19
90	Hydrated Electron Production by Reaction of Hydrogen Atoms with Hydroxide Ions: A First-Principles Molecular Dynamics Study. Journal of Physical Chemistry A, 2008, 112, 7027-7034.	1.1	18

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91	Infrared spectroscopy of small protonated water clusters at room temperature: An effective modes analysis. Journal of Chemical Physics, 2011, 134, 084302.	1.2	18
92	An Ab Initio Molecular Dynamics Study on the Hydrolysis of the Po(IV) Aquaion in Water. Journal of Physical Chemistry B, 2010, 114, 12866-12874.	1.2	17
93	Vibrational dynamics of zero-field-splitting hamiltonian in gadolinium-based MRI contrast agents from ab initio molecular dynamics. Journal of Chemical Physics, 2014, 141, 014201.	1.2	16
94	The MgCO3â€“CaCO3â€“Li2CO3â€“Na2CO3â€“K2CO3 melts: Thermodynamics and transport properties by atomistic simulations. Journal of Chemical Physics, 2019, 150, 214503.	1.2	16
95	Atomistic simulations of molten carbonates: Thermodynamic and transport properties of the Li2CO3â€”Na2CO3â€”K2CO3 system. Journal of Chemical Physics, 2019, 150, 094504.	1.2	16
96	Mass-zero constrained molecular dynamics for electrode charges in simulations of electrochemical systems. Journal of Chemical Physics, 2020, 152, 194701.	1.2	16
97	Computing thermal Wigner densities with the phase integration method. Journal of Chemical Physics, 2014, 141, 084102.	1.2	15
98	Hydration properties of lanthanoid(iii) carbonate complexes in liquid water determined by polarizable molecular dynamics simulations. Physical Chemistry Chemical Physics, 2014, 16, 3693.	1.3	15
99	Ca²⁺â€Cl^{â^'} Association in Water Revisited: the Role of Cation Hydration. ChemPhysChem, 2017, 18, 2807-2811.	1.0	15
100	Adiabatic motion and statistical mechanics via mass-zero constrained dynamics. Physical Chemistry Chemical Physics, 2020, 22, 10775-10785.	1.3	15
101	The important role of non-covalent interactions for the vibrational circular dichroism of lactic acid in aqueous solution. Physical Chemistry Chemical Physics, 2021, 23, 17232-17241.	1.3	15
102	Wavefunction quantization of the proton motion in a H5O2+ dimer solvated in liquid water. Journal of Molecular Structure, 2000, 552, 117-136.	1.8	13
103	Initial metalâ€“metal bond breakage detected by fs X-ray scattering in the photolysis of Ru3(CO)12 in cyclohexane at 400 nm. Photochemical and Photobiological Sciences, 2019, 18, 319-327.	1.6	13
104	The trisulfur radical ion S ₃ ^{â€¢â^'} controls platinum transport by hydrothermal fluids. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	13
105	Electronic redistribution around oxygen atoms in silicate melts by ab initio molecular dynamics simulation. Journal of Non-Crystalline Solids, 2011, 357, 2555-2561.	1.5	12
106	Computing three-dimensional densities from force densities improves statistical efficiency. Journal of Chemical Physics, 2019, 151, 064124.	1.2	12
107	Theoretical investigation of the ultrafast dissociation of core-ionized water and uracil molecules immersed in liquid water. European Physical Journal D, 2010, 60, 77-83.	0.6	10
108	Theoretical study of the ionization of liquid water from its several initial orbitals by fast electron impact. Journal of Physics B: Atomic, Molecular and Optical Physics, 2015, 48, 155201.	0.6	10

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109	Investigation of the fragmentation of core-ionised deoxyribose: a study as a function of the tautomeric form. Physical Chemistry Chemical Physics, 2015, 17, 32375-32383.	1.3	10
110	An ab initio CASSCF study of zero field splitting fluctuations in the octet ground state of aqueous [Gd(iii)(HPDO3A)(H2O)]. Journal of Chemical Physics, 2017, 147, 244306.	1.2	10
111	Structure of the Photodissociation Products of CCl4, CBr4, and Cl4in Solution Studied by DFT and ab Initio Calculations. Journal of Physical Chemistry A, 2006, 110, 11178-11187.	1.1	9
112	Density Functional Theory Based Ab Initio Molecular Dynamics Using the Car-Parrinello Approach. , 2006, , 223-285.		9
113	Infrared spectroscopy and effective modes analysis of the protonated water dimer H+(H2O)2 at room temperature under H/D substitution. Journal of Chemical Physics, 2011, 134, 084303.	1.2	9
114	Direct observation of the substitution effects on the hydrogen bridge dynamics in selected Schiff basesâ€"A comparative molecular dynamics study. Journal of Chemical Physics, 2011, 134, 034308.	1.2	9
115	Varying the charge of small cations in liquid water: Structural, transport, and thermodynamical properties. Journal of Chemical Physics, 2012, 137, 164501.	1.2	9
116	Hyperfine interactions in a gadolinium-based MRI contrast agent: High-frequency modulations from ab initio simulations. Journal of Chemical Physics, 2013, 139, 104115.	1.2	9
117	Probing anharmonic phonons by quantum correlators: A path integral approach. Journal of Chemical Physics, 2021, 154, 224108.	1.2	9
118	Liquid water ionization by fast electron impact: a multiple differential study for the 1B1orbital. Journal of Physics B: Atomic, Molecular and Optical Physics, 2012, 45, 045206.	0.6	8
119	Transient hydrodynamic finite-size effects in simulations under periodic boundary conditions. Physical Review E, 2017, 95, 061301.	0.8	8
120	Gold speciation in hydrothermal fluids revealed by in situ high energy resolution X-ray absorption spectroscopy. American Mineralogist, 2022, 107, 369-376.	0.9	8
121	Electronic control of reactivity using density functional perturbation methods. Chemical Physics Letters, 2002, 365, 305-312.	1.2	7
122	Ultrafast nonadiabatic fragmentation dynamics of biomolecules. Journal of Physics: Conference Series, 2014, 488, 012037.	0.3	7
123	Microscopic flow around a diffusing particle. Journal of Chemical Physics, 2017, 147, 094502.	1.2	7
124	TDDFT and Quantum-Classical Dynamics: A Universal Tool Describing the Dynamics of Matter. , 2018, , 1-47.		7
125	Deciphering second harmonic generation signals. Chemical Science, 2021, 12, 15134-15142.	3.7	7
126	An Adiabatic Linearized Path Integral Approach for Quantum Time-Correlation Functions II:Â A Cumulant Expansion Method for Improving Convergence. Journal of Physical Chemistry B, 2006, 110, 16026-16034.	1.2	6

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127	Carbon species solvated in molten carbonate electrolyser cell from first-principles simulations. International Journal of Hydrogen Energy, 2021, 46, 15008-15023.	3.8	6
128	Proton Collision on Deoxyribose Originating from Doubly Ionized Water Molecule Dissociation. Journal of Physical Chemistry A, 2018, 122, 5311-5320.	1.1	5
129	Spontaneous liquid water dissociation on hybridised boron nitride and graphene atomic layers from ab initio molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 10710-10716.	1.3	5
130	Frontiers in molecular simulation of solvated ions, molecules and interfaces. Physical Chemistry Chemical Physics, 2020, 22, 10393-10396.	1.3	5
131	Gas phase infrared spectra from quasi-classical Kubo time correlation functions. Molecular Physics, 2015, 113, 2894-2904.	0.8	4
132	Roles of Hydration for Inducing Decomposition of 2-Deoxy-d-ribose by Ionization of Oxygen K-Shell Electrons. Radiation Research, 2018, 189, 264-272.	0.7	4
133	VCDâ€VerstÃrkung durch chirale Packungseffekte in molekularen Kristallen. Angewandte Chemie, 2018, 130, 13528-13532.	1.6	4
134	Reactivity of an Excess Electron with Monovalent Cations in Bulk Water by Mixed Quantum Classical Molecular Dynamics Simulations. Molecular Simulation, 2004, 30, 749-754.	0.9	3
135	Time-resolved x-ray diffraction from small molecules in solution. , 2004, , 337-347.		3
136	Unexpected remote effect in red fluorescent sensors based on extended APTRA. Tetrahedron, 2013, 69, 10482-10487.	1.0	3
137	Developing polarizable potential for molecular dynamics of Cm(III)-carbonate complexes in liquid water. Journal of Molecular Modeling, 2014, 20, 2398.	0.8	3
138	Gas phase infrared spectra via the phase integration quasi-classical method. Molecular Simulation, 2014, 40, 196-207.	0.9	3
139	Maximum probability domains for the analysis of the microscopic structure of liquids. Journal of Chemical Physics, 2015, 142, 064117.	1.2	3
140	TDDFT and Quantum-Classical Dynamics: A Universal Tool Describing the Dynamics of Matter. , 2018, , 1-47.		3
141	TDDFT and Quantum-Classical Dynamics: A Universal Tool Describing the Dynamics of Matter. , 2020, , 75-121.		3
142	Why Local and Non-local Terms are Essential for Second Harmonic Generation Simulation?. Physical Chemistry Chemical Physics, 2022, , .	1.3	3
143	Quantum RÃ©nyi entropy by optimal thermodynamic integration paths. Physical Review Research, 2022, 4, .	1.3	3
144	Ionization of liquid water by fast electron impact: multiple differential cross sections for the 1B1orbital. Journal of Physics: Conference Series, 2011, 288, 012010.	0.3	2

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145	Model potentials in liquid water ionization by fast electron impact. Journal of Physics: Conference Series, 2015, 583, 012023.	0.3	2
146	Double differential cross sections for liquid water ionization by fast electron impact. European Physical Journal D, 2017, 71, 1.	0.6	2
147	Ab Initio Molecular Dynamics Simulations to Interpret the Molecular Fragmentation Induced in Deoxyribose by Synchrotron Soft X-Rays. Quantum Beam Science, 2019, 3, 24.	0.6	2
148	A first-principles computational comparison of defect-free and disordered, fluorinated anatase TiO2 (001) interfaces with water. RSC Advances, 2020, 10, 8982-8988.	1.7	2
149	Real Time Visualization of Atomic Motions in Dense Phases. , 2004, , 111-128.		2
150	Determination of structure in liquid solutions - implications for picosecond photoexcitation studies. Journal of Physics Condensed Matter, 2003, 15, S137-S143.	0.7	1
151	Ultrafast non-adiabatic fragmentation dynamics of doubly charged uracil in gas and liquid phase. Journal of Physics: Conference Series, 2012, 388, 102055.	0.3	1
152	p of silicic acid in presence of La³⁺using single sweep method coupled to DFT-based molecular dynamics. Molecular Physics, 2013, 111, 3478-3485.	0.8	1
153	Atomic partial charges in condensed phase from an exact sum rule for infrared absorption. Molecular Physics, 2014, 112, 1457-1462.	0.8	1
154	Solvation dynamics of coumarin 153 in benzene-acetonitrile and benzene-methanol mixtures: a Molecular Dynamics study. , 2004, , 245-248.		0
155	Electronic Structure and Solvation of Copper and Silver Ions: A Theoretical Picture of a Model Aqueous Redox Reaction. ChemInform, 2004, 35, no.	0.1	0
156	Differential cross sections for single ionization of water molecules in liquid phase by electron impact at high impact energies. Journal of Physics: Conference Series, 2009, 194, 052027.	0.3	0
157	Ionization of water clusters by fast Highly Charged Ions: Stability, fragmentation, energetics and charge mobility. Journal of Physics: Conference Series, 2009, 194, 102032.	0.3	0
158	Ultrafast dissociation of a core-ionized water molecule in liquid phase: Density functional theory based simulations. Journal of Physics: Conference Series, 2009, 194, 102027.	0.3	0
159	Multiple differential cross sections for the ionization of liquid water molecules by fast electron impact. Journal of Physics: Conference Series, 2012, 388, 052064.	0.3	0
160	Triple differential cross sections for liquid water ionization by impact of fast electrons. Journal of Physics: Conference Series, 2014, 488, 052024.	0.3	0
161	Double differential cross sections for liquid water ionization by impact of fast electrons. Journal of Physics: Conference Series, 2015, 635, 072061.	0.3	0
162	RÃ¼cktitelbild: VCDâ€VerstÃrkung durch chirale Packungseffekte in molekularen Kristallen (Angew.) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.6	0

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163	A guide to statistical physics issues in molecular simulations. Ã‰cole ThÃ©matique De La SociÃ©tÃ© FranÃ§aise De La Neutronique, 2011, 12, 15-30.	0.2	0
164	Visualizing Chemical Reactions with X-rays. Ukrainian Journal of Physics, 2022, 56, 763.	0.1	0