Ivano Tavernelli

List of Publications by Year
in descending order

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167 papers	13,870 citations	30551 56 h-index	24511 114 g-index
172 all docs	172 docs citations	172 times ranked	16062 citing authors

#	Article	IF	Citations
1	Coarse-grained intermolecular interactions on quantum processors. Physical Review A, 2022, 105, .	1.0	3
2	Quantum neural networks force fields generation. Machine Learning: Science and Technology, 2022, 3, 035004.	2.4	5
3	Ancilla-free implementation of generalized measurements for qubits embedded in a qudit space. Physical Review Research, 2022, 4, .	1.3	14
4	A proposal for using molecular spin qudits as quantum simulators of lightâ€“matter interactions. Journal of Materials Chemistry C, 2021, 9, 10266-10275.	2.7	23
5	Quantum algorithm for alchemical optimization in material design. Chemical Science, 2021, 12, 4345-4352.	3.7	14
6	Variationalâ€‰Learningâ€‰forâ€‰Quantumâ€‰Artificial Neural Networks. IEEE Transactions on Quantum Engineering, 2021, 2, 1-10.	2.9	19
7	Microcanonical and finite-temperature ab initio molecular dynamics simulations on quantum computers. Physical Review Research, 2021, 3, .	1.3	26
8	Resource-efficient quantum algorithm for protein folding. Npj Quantum Information, 2021, 7, .	2.8	62
9	Quantum HF/DFT-embedding algorithms for electronic structure calculations: Scaling up to complex molecular systems. Journal of Chemical Physics, 2021, 154, 114105.	1.2	29
10	Probing Molecular Excited States by Atomic Force Microscopy. Physical Review Letters, 2021, 126, 176801.	2.9	9
11	Gravitational Quantum Dynamics: A Geometrical Perspective. Foundations of Physics, 2021, 51, 1.	0.6	3
12	Quantum-optimal-control-inspired ansatz for variational quantum algorithms. Physical Review Research, 2021, 3, .	1.3	37
13	Improved Accuracy on Noisy Devices by Nonunitary Variational Quantum Eigensolver for Chemistry Applications. Journal of Chemical Theory and Computation, 2021, 17, 3946-3954.	2.3	9
14	Assessing the Nature of Chiral-Induced Spin Selectivity by Magnetic Resonance. Journal of Physical Chemistry Letters, 2021, 12, 6341-6347.	2.1	25
15	Simulating Static and Dynamic Properties of Magnetic Molecules with Prototype Quantum Computers. Magnetochemistry, 2021, 7, 117.	1.0	14
16	Learning to Measure: Adaptive Informationally Complete Generalized Measurements for Quantum Algorithms. PRX Quantum, 2021, 2, .	3.5	37
17	Molecular Quantum Dynamics: A Quantum Computing Perspective. Accounts of Chemical Research, 2021, 54, 4229-4238.	7.6	33
18	Quantum algorithms for quantum dynamics: A performance study on the spin-boson model. Physical Review Research, 2021, 3, .	1.3	17

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19	Redox Properties of Native and Damaged DNA from Mixed Quantum Mechanical/Molecular Mechanics Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 6690-6701.	2.3	15
20	Quantum equilibration of the double-proton transfer in a model system porphine. Physical Chemistry Chemical Physics, 2020, 22, 22332-22341.	1.3	0
21	Charge Separation and Charge Carrier Mobility in Photocatalytic Metalâ€Organic Frameworks. Advanced Functional Materials, 2020, 30, 2003792.	7.8	64
22	Optical absorption properties of metalâ€“organic frameworks: solid state versus molecular perspective. Physical Chemistry Chemical Physics, 2020, 22, 19512-19521.	1.3	14
23	Toward scalable simulations of lattice gauge theories on quantum computers. Physical Review D, 2020, 102, .	1.6	38
24	Hardware efficient quantum algorithms for vibrational structure calculations. Chemical Science, 2020, 11, 6842-6855.	3.7	50
25	Energy-based descriptors for photo-catalytically active metalâ€“organic framework discovery. Journal of Materials Chemistry A, 2020, 8, 4473-4482.	5.2	24
26	Quantum orbital-optimized unitary coupled cluster methods in the strongly correlated regime: Can quantum algorithms outperform their classical equivalents?. Journal of Chemical Physics, 2020, 152, 124107.	1.2	91
27	Correlation effects in parallel tempering and the role of the swapping frequency. Physical Chemistry Chemical Physics, 2020, 22, 10802-10806.	1.3	0
28	Insights into the Electronic Properties and Charge Transfer Mechanism of a Porphyrin Ruthenium-Based Metalâ€“Organic Framework. Chemistry of Materials, 2020, 32, 4194-4204.	3.2	31
29	TDDFT and Quantum-Classical Dynamics: A Universal Tool Describing the Dynamics of Matter. , 2020, , 75-121.		3
30	Quantum implementation of an artificial feed-forward neural network. Quantum Science and Technology, 2020, 5, 044010.	2.6	46
31	Nonadiabatic Molecular Quantum Dynamics with Quantum Computers. Physical Review Letters, 2020, 125, 260511.	2.9	42
32	Variational quantum simulation of ultrastrong light-matter coupling. Physical Review Research, 2020, 2, .	1.3	16
33	Quantum equation of motion for computing molecular excitation energies on a noisy quantum processor. Physical Review Research, 2020, 2, .	1.3	110
34	Variational learning for quantum artificial neural networks. , 2020, , .		12
35	Nonunitary Operations for Ground-State Calculations in Near-Term Quantum Computers. Physical Review Letters, 2019, 123, 130501.	2.9	31
36	Vertical Ionization Energies and Electron Affinities of Native and Damaged DNA Bases, Nucleotides, and Pairs from Density Functional Theory Calculations: Model Assessment and Implications for DNA Damage Recognition and Repair. Journal of Chemical Theory and Computation, 2019, 15, 2042-2052.	2.3	19

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37	Gate-Efficient Simulation of Molecular Eigenstates on a Quantum Computer. Physical Review Applied, 2019, 11, .	1.5	104
38	Quantum hardware simulating four-dimensional inelastic neutron scattering. Nature Physics, 2019, 15, 455-459.	6.5	89
39	Charge migration in photo-ionized aromatic amino acids. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20170472.	1.6	15
40	On the self-interference in electron scattering: Copenhagen, Bohmian and geometrical interpretations of quantum mechanics. Annals of Physics, 2018, 393, 447-465.	1.0	6
41	Quantum modeling of ultrafast photoinduced charge separation. Journal of Physics Condensed Matter, 2018, 30, 013002.	0.7	29
42	TDDFT and Quantum-Classical Dynamics: A Universal Tool Describing the Dynamics of Matter. , 2018, , 1-47.		3
43	TDDFT and Quantum-Classical Dynamics: A Universal Tool Describing the Dynamics of Matter. , 2018, , 1-47.		7
44	Proton Collision on Deoxyribose Originating from Doubly Ionized Water Molecule Dissociation. Journal of Physical Chemistry A, 2018, 122, 5311-5320.	1.1	5
45	Vibrational coherence transfer in the ultrafast intersystem crossing of a diplatinum complex in solution. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E6396-E6403.	3.3	51
46	Attosecond Pumpâ€“Probe Spectroscopy of Charge Dynamics in Tryptophan. Journal of Physical Chemistry Letters, 2018, 9, 4570-4577.	2.1	74
47	Nuclear quantum effects in electronic (non)adiabatic dynamics. European Physical Journal B, 2018, 91, 1.	0.6	28
48	CT-MQC â€“ a coupled-trajectory mixed quantum/classical method including nonadiabatic quantum coherence effects. European Physical Journal B, 2018, 91, 1.	0.6	37
49	Quantum algorithms for electronic structure calculations: Particle-hole Hamiltonian and optimized wave-function expansions. Physical Review A, 2018, 98, .	1.0	214
50	Quantum optimization using variational algorithms on near-term quantum devices. Quantum Science and Technology, 2018, 3, 030503.	2.6	411
51	TDDFT-Based Spinâ€“Orbit Couplings of 0D, 1D, and 2D Carbon Nanostructures: Static and Dynamical Effects. Journal of Physical Chemistry C, 2017, 121, 10140-10152.	1.5	8
52	Role of electron-nuclear coupled dynamics on charge migration induced by attosecond pulses in glycine. Chemical Physics Letters, 2017, 683, 357-364.	1.2	34
53	Ab Initio Nonadiabatic Dynamics with Coupled Trajectories: A Rigorous Approach to Quantum (De)Coherence. Journal of Physical Chemistry Letters, 2017, 8, 3048-3055.	2.1	123
54	Photophysics of a copper phenanthroline elucidated by trajectory and wavepacket-based quantum dynamics: a synergetic approach. Physical Chemistry Chemical Physics, 2017, 19, 19590-19600.	1.3	48

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55	Tris-heteroleptic Iridium Complexes Based on Cyclometalated Ligands with Different Cores. Inorganic Chemistry, 2017, 56, 11565-11576.	1.9	23
56	Characterization of the Photochemical Properties of 5-Benzyluracil via Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2017, 121, 3909-3917.	1.1	15
57	Universal steps in quantum dynamics with time-dependent potential-energy surfaces: Beyond the Born-Oppenheimer picture. Physical Review A, 2016, 94, .	1.0	10
58	Optimizing qubit resources for quantum chemistry simulations in second quantization on a quantum computer. Journal of Physics A: Mathematical and Theoretical, 2016, 49, 295301.	0.7	47
59	On the geometrization of quantum mechanics. Annals of Physics, 2016, 371, 239-253.	1.0	16
60	Decoherence, control and attosecond probing of XUV-induced charge migration in biomolecules. A theoretical outlook. Faraday Discussions, 2016, 194, 41-59.	1.6	43
61	Nonadiabatic dynamics with intersystem crossings: A time-dependent density functional theory implementation. Journal of Chemical Physics, 2015, 143, 224105.	1.2	52
62	Nonadiabatic Molecular Dynamics Simulations: Synergies between Theory and Experiments. Accounts of Chemical Research, 2015, 48, 792-800.	7.6	87
63	Theoretical Rationalization of the Emission Properties of Prototypical Cu(I)â€“Phenanthroline Complexes. Journal of Physical Chemistry A, 2015, 119, 7026-7037.	1.1	45
64	In Situ Mapping of the Molecular Arrangement of Amphiphilic Dye Molecules at the TiO₂ Surface of Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2015, 7, 10834-10842.	4.0	30
65	Conditional Bornâ€“Oppenheimer Dynamics: Quantum Dynamics Simulations for the Model Porphine. Journal of Physical Chemistry Letters, 2015, 6, 1529-1535.	2.1	21
66	Local Control Theory in Trajectory Surface Hopping Dynamics Applied to the Excitedâ€State Proton Transfer of 4â€Hydroxyacridine. ChemPhysChem, 2015, 16, 2127-2133.	1.0	9
67	Probing wavepacket dynamics using ultrafast x-ray spectroscopy. Journal of Physics B: Atomic, Molecular and Optical Physics, 2015, 48, 214001.	0.6	46
68	Study of the Redox Properties of Singlet and Triplet Tris(2,2â€²-bipyridine)ruthenium(II) ([Ru(bpy)₃]²⁺) in Aqueous Solution by Full Quantum and Mixed Quantum/Classical Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2014, 118, 3950-3959.	1.2	19
69	Nonadiabatic Molecular Dynamics Based on Trajectories. Entropy, 2014, 16, 62-85.	1.1	46
70	Derivation of spin-orbit couplings in collinear linear-response TDDFT: A rigorous formulation. Journal of Chemical Physics, 2014, 140, 144103.	1.2	47
71	Probing the electronic and geometric structure of ferric and ferrous myoglobins in physiological solutions by Fe K-edge absorption spectroscopy. Physical Chemistry Chemical Physics, 2014, 16, 1617-1631.	1.3	39
72	Dye-sensitized solar cells with 13% efficiency achieved through the molecular engineering of porphyrin sensitizers. Nature Chemistry, 2014, 6, 242-247.	6.6	3,982

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73	Origin of the Spectral Shifts among the Early Intermediates of the Rhodopsin Photocycle. Journal of the American Chemical Society, 2014, 136, 3842-3851.	6.6	42
74	X-ray Spectroscopic Study of Solvent Effects on the Ferrous and Ferric Hexacyanide Anions. Journal of Physical Chemistry A, 2014, 118, 9411-9418.	1.1	42
75	Generalized QM/MM Force Matching Approach Applied to the 11-cis Protonated Schiff Base Chromophore of Rhodopsin. Journal of Chemical Theory and Computation, 2014, 10, 412-422.	2.3	21
76	A Quantum Dynamics Study of the Ultrafast Relaxation in a Prototypical Cu(I)â€“Phenanthroline. Journal of Physical Chemistry A, 2014, 118, 9861-9869.	1.1	74
77	Photophysics and Photochemistry of a DNAâ€“Protein Cross-Linking Model: A Synergistic Approach Combining Experiments and Theory. Journal of Physical Chemistry B, 2014, 118, 4983-4992.	1.2	15
78	Structureâ€“property relationships based on Hammett constants in cyclometalated iridium(<scp>iii</scp>) complexes: their application to the design of a fluorine-free FIrPic-like emitter. Dalton Transactions, 2014, 43, 5667-5679.	1.6	96
79	A Vibronic Coupling Hamiltonian to Describe the Ultrafast Excited State Dynamics of a Cu(I)-Phenanthroline Complex. Chimia, 2014, 68, 227.	0.3	35
80	Assessing the performance of computational methods for the prediction of the ground state structure of a cyclic decapeptide. International Journal of Quantum Chemistry, 2013, 113, 808-814.	1.0	14
81	The role of Hartreeâ€“Fock exchange in the simulation of X-ray absorption spectra: A study of photoexcited. Chemical Physics Letters, 2013, 580, 179-184.	1.2	43
82	Ultrafast Damage Following Radiationâ€Induced Oxidation of Uracil in Aqueous Solution. Angewandte Chemie - International Edition, 2013, 52, 3160-3163.	7.2	34
83	Rhodopsin Absorption from First Principles: Bypassing Common Pitfalls. Journal of Chemical Theory and Computation, 2013, 9, 2441-2454.	2.3	81
84	Nonadiabatic ab initio molecular dynamics using linear-response time-dependent density functional theory. Open Physics, 2013, 11, .	0.8	6
85	Photodynamics of Lys+-Trp protein motifs: Hydrogen bonds ensure photostability. Faraday Discussions, 2013, 163, 189.	1.6	7
86	In situparameterisation of SCC-DFTB repulsive potentials by iterative Boltzmann inversion. Molecular Physics, 2013, 111, 3595-3607.	0.8	28
87	X-ray Absorption Spectroscopy of Ground and Excited Rheniumâ€“Carbonylâ€“Diimine Complexes: Evidence for a Two-Center Electron Transfer. Journal of Physical Chemistry A, 2013, 117, 361-369.	1.1	63
88	Intricacies of Describing Weak Interactions Involving Halogen Atoms within Density Functional Theory. Journal of Chemical Theory and Computation, 2013, 9, 955-964.	2.3	24
89	Solvent rearrangements during the transition from hydrophilic to hydrophobic solvation. Chemical Physics, 2013, 410, 25-30.	0.9	10
90	Trajectoryâ€Based Nonadiabatic Dynamics with Timeâ€Dependent Density Functional Theory. ChemPhysChem, 2013, 14, 1314-1340.	1.0	168

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91	Molecular Engineering of a Fluorene Donor for Dye-Sensitized Solar Cells. Chemistry of Materials, 2013, 25, 2733-2739.	3.2	154
92	Unravelling the Potential for Dithienopyrrole Sensitizers in Dye-Sensitized Solar Cells. Chemistry of Materials, 2013, 25, 2642-2648.	3.2	49
93	On trajectory-based nonadiabatic dynamics: Bohmian dynamics versus trajectory surface hopping. Journal of Chemical Physics, 2013, 138, 184112.	1.2	62
94	Solvent-Induced Luminescence Quenching: Static and Time-Resolved X-Ray Absorption Spectroscopy of a Copper(I) Phenanthroline Complex. Journal of Physical Chemistry A, 2013, 117, 4591-4601.	1.1	111
95	The Charge Transfer Problem in Density Functional Theory Calculations of Aqueously Solvated Molecules. Journal of Physical Chemistry B, 2013, 117, 12189-12201.	1.2	92
96	Two Misfolding Routes for the Prion Protein around pH 4.5. PLoS Computational Biology, 2013, 9, e1003057.	1.5	18
97	Local Control Theory using Trajectory Surface Hopping and Linear-Response Time-Dependent Density Functional Theory. Chimia, 2013, 67, 218-221.	0.3	6
98	Ultrafast anisotropic x-ray scattering in the condensed phase. New Journal of Physics, 2012, 14, 113002.	1.2	11
99	Hydrophobicity with atomic resolution: Steady-state and ultrafast X-ray absorption and molecular dynamics studies. Pure and Applied Chemistry, 2012, 85, 53-60.	0.9	6
100	Excited State Dynamics with Quantum Trajectories. Chimia, 2012, 66, 174.	0.3	5
101	Acid-Induced Degradation of Phosphorescent Dopants for OLEDs and Its Application to the Synthesis of Tris-heteroleptic Iridium(III) Bis-cyclometalated Complexes. Inorganic Chemistry, 2012, 51, 215-224.	1.9	165
102	Simulations of X-ray absorption spectra: the effect of the solvent. Physical Chemistry Chemical Physics, 2012, 14, 9444.	1.3	25
103	Structure and Dynamics of Liquid Water from ab Initio Molecular Dynamicsâ€"Comparison of BLYP, PBE, and revPBE Density Functionals with and without van der Waals Corrections. Journal of Chemical Theory and Computation, 2012, 8, 3902-3910.	2.3	247
104	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
105	Nanocomposites Containing Neutral Blue Emitting Cyclometalated Iridium(III) Emitters for Oxygen Sensing. Chemistry of Materials, 2012, 24, 2330-2338.	3.2	63
106	Influence of Halogen Atoms on a Homologous Series of Bis-Cyclometalated Iridium(III) Complexes. Inorganic Chemistry, 2012, 51, 799-811.	1.9	107
107	A Simple Approach to Room Temperature Phosphorescent Allenylidene Complexes. Angewandte Chemie - International Edition, 2012, 51, 8030-8033.	7.2	20
108	Integrating computational methods to retrofit enzymes to synthetic pathways. Biotechnology and Bioengineering, 2012, 109, 572-582.	1.7	32

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109	Structure and Dynamics of Liquid Water from ab Initio Molecular Dynamicsâ€"Comparison of BLYP, PBE, and revPBE Density Functionals with and without van der Waals Corrections. Journal of Chemical Theory and Computation, 2012, 8, 3902-3910.	2.3	116
110	Trajectory-based solution of the nonadiabatic quantum dynamics equations: an on-the-fly approach for molecular dynamics simulations. Physical Chemistry Chemical Physics, 2011, 13, 3231.	1.3	64
111	Probing the Transition from Hydrophilic to Hydrophobic Solvation with Atomic Scale Resolution. Journal of the American Chemical Society, 2011, 133, 12740-12748.	6.6	71
112	Mechanical (QM/MM) Simulations of Adiabatic and Nonadiabatic Ultrafast Phenomena. Chimia, 2011, 65, 330-333.	0.3	5
113	Nonadiabatic molecular dynamics with solvent effects: A LR-TDDFT QM/MM study of ruthenium (II) tris (bipyridine) in water. Chemical Physics, 2011, 391, 101-109.	0.9	101
114	Coldâ€Ion Spectroscopy Reveals the Intrinsic Structure of a Decapeptide. Angewandte Chemie - International Edition, 2011, 50, 5383-5386.	7.2	63
115	Pushing the Frontiers of First-Principles Based Computer Simulations of Chemical and Biological Systems. Chimia, 2011, 65, 667.	0.3	22
116	Ultrafast Nonadiabatic Fragmentation Dynamics of Doubly Charged Uracil in a Gas Phase. Physical Review Letters, 2011, 107, 023202.	2.9	63
117	Predicting Novel Binding Modes of Agonists to Î² Adrenergic Receptors Using All-Atom Molecular Dynamics Simulations. PLoS Computational Biology, 2011, 7, e1001053.	1.5	38
118	Electron Localization Dynamics in the Triplet Excited State of [Ru(bpy)₃]²⁺ in Aqueous Solution. Chemistry - A European Journal, 2010, 16, 5889-5894.	1.7	68
119	The solvent shell structure of aqueous iodide: X-ray absorption spectroscopy and classical, hybrid QM/MM and full quantum molecular dynamics simulations. Chemical Physics, 2010, 371, 24-29.	0.9	56
120	Nonadiabatic coupling vectors for excited states within time-dependent density functional theory in the Tammâ€"Dancoff approximation and beyond. Journal of Chemical Physics, 2010, 133, 194104.	1.2	105
121	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
122	A Conserved Protonation-Induced Switch can Trigger â€œIonic-Lockâ€•Formation in Adrenergic Receptors. Journal of Molecular Biology, 2010, 397, 1339-1349.	2.0	36
123	On nonadiabatic coupling vectors in time-dependent density functional theory. Journal of Chemical Physics, 2009, 131, 196101.	1.2	80
124	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
125	Non-adiabatic dynamics using time-dependent density functional theory: Assessing the coupling strengths. Computational and Theoretical Chemistry, 2009, 914, 22-29.	1.5	61
126	Dispersion Corrected Atom-Centered Potentials for Phosphorus. Journal of Chemical Theory and Computation, 2009, 5, 2930-2934.	2.3	15

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127	Ab Initio Excited State Properties and Dynamics of a Prototype Ïƒ-Bridged-Donorâ^'Acceptor Molecule. Journal of Physical Chemistry A, 2009, 113, 9595-9602.	1.1	21
128	New Paradigm in Molecular Engineering of Sensitizers for Solar Cell Applications. Journal of the American Chemical Society, 2009, 131, 5930-5934.	6.6	385
129	Importance of van der Waals Interactions in Liquid Water. Journal of Physical Chemistry B, 2009, 113, 1127-1131.	1.2	175
130	Binding of Organometallic Ruthenium(II) Anticancer Compounds to Nucleobases: A Computational Study. Journal of Physical Chemistry A, 2009, 113, 11888-11897.	1.1	34
131	On the proton transfer mechanism in ammonia-bridged 7-hydroxyquinoline: a TDDFT molecular dynamics study. Physical Chemistry Chemical Physics, 2009, 11, 4549.	1.3	26
132	Nonadiabatic coupling vectors within linear response time-dependent density functional theory. Journal of Chemical Physics, 2009, 130, 124107.	1.2	114
133	Combined QM/MM and Classical Molecular Dynamics Study of [Ru(bpy)₃]²⁺ in Water. Journal of Physical Chemistry B, 2009, 113, 7737-7744.	1.2	61
134	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
135	Timeâ€Dependent Density Functional Theory Molecular Dynamics Simulations of Liquid Water Radiolysis. ChemPhysChem, 2008, 9, 2099-2103.	1.0	45
136	Computational Study of Thymine Dimer Radical Anion Splitting in the Self-Repair Process of Duplex DNA. Journal of the American Chemical Society, 2008, 130, 3443-3450.	6.6	63
137	Mixed time-dependent density-functional theory/classical trajectory surface hopping study of oxirane photochemistry. Journal of Chemical Physics, 2008, 129, 124108.	1.2	182
138	DNA Structural Distortions Induced by Rutheniumâ^'Arene Anticancer Compounds. Journal of the American Chemical Society, 2008, 130, 10921-10928.	6.6	94
139	Trajectory Surface Hopping within Linear Response Time-Dependent Density-Functional Theory. Physical Review Letters, 2007, 98, 023001.	2.9	324
140	Early stages of radiation damage in graphite and carbon nanostructures: A first-principles molecular dynamics study. Physical Review B, 2007, 75, .	1.1	68
141	NMR Solvent Shifts of Adenine in Aqueous Solution from Hybrid QM/MM Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2007, 111, 5225-5232.	1.2	34
142	Predicting Noncovalent Interactions between Aromatic Biomolecules with London-Dispersion-Corrected DFT. Journal of Physical Chemistry B, 2007, 111, 14346-14354.	1.2	62
143	Optical Spectra of Cu(II)â^'Azurin by Hybrid TDDFT-Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2007, 111, 10248-10252.	1.2	38
144	Structural and Energetic Properties of Organometallic Ruthenium(II) Diamine Anticancer Compounds and Their Interaction with Nucleobases. Journal of Chemical Theory and Computation, 2007, 3, 1212-1222.	2.3	25

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145	Self-Interaction Corrected Density Functional Theory for the Study of Intramolecular Electron Transfer Dynamics in Radical Carbocations. Journal of Physical Chemistry A, 2007, 111, 13528-13536.	1.1	10
146	Weakly Bonded Complexes of Aliphatic and Aromatic Carbon Compounds Described with Dispersion Corrected Density Functional Theory. Journal of Chemical Theory and Computation, 2007, 3, 1673-1679.	2.3	66
147	Microsolvation Effects on the Excited-State Dynamics of Protonated Tryptophan. Journal of the American Chemical Society, 2006, 128, 16938-16943.	6.6	144
148	Influence of Hydrogen-Bonding Substituents on the Cytotoxicity of RAPTA Compounds. Organometallics, 2006, 25, 756-765.	1.1	154
149	A Novel Hamiltonian Replica Exchange MD Protocol to Enhance Protein Conformational Space Sampling. Journal of Chemical Theory and Computation, 2006, 2, 217-228.	2.3	123
150	Diabatic free energy curves and coordination fluctuations for the aqueous Ag+âˆ•Ag2+ redox couple: A biased Born-Oppenheimer molecular dynamics investigation. Journal of Chemical Physics, 2006, 124, 064507.	1.2	112
151	Role of protein frame and solvent for the redox properties of azurin from Pseudomonas aeruginosa. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 19641-19646.	3.3	135
152	Electronic density response of liquid water using time-dependent density functional theory. Physical Review B, 2006, 73, .	1.1	63
153	Quantum Mechanical/Molecular Mechanical (QM/MM) Car-Parrinello Simulations in Excited States. Chimia, 2005, 59, 493-498.	0.3	34
154	Rational Design of Organo-Ruthenium Anticancer Compounds. Chimia, 2005, 59, 81-84.	0.3	33
155	Density-functional molecular-dynamics study of the redox reactions of two anionic, aqueous transition-metal complexes. Journal of Chemical Physics, 2005, 122, 234505.	1.2	86
156	Binding of Organometallic Ruthenium(II) and Osmium(II) Complexes to an Oligonucleotide:Â A Combined Mass Spectrometric and Theoretical Studyâ€. Organometallics, 2005, 24, 2114-2123.	1.1	210
157	Molecular dynamics in electronically excited states using time-dependent density functional theory. Molecular Physics, 2005, 103, 963-981.	0.8	130
158	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
159	Optimization of Effective Atom Centered Potentials for London Dispersion Forces in Density Functional Theory. Physical Review Letters, 2004, 93, 153004.	2.9	489
160	Dynamics of RNase-A and S-Protein: A Molecular Dynamics Simulation of the Transition Toward a Folding Intermediate. Biophysical Journal, 2003, 85, 2633-2640.	0.2	9
161	Protein Dynamics, Thermal Stability, and Free-Energy Landscapes: A Molecular Dynamics Investigation. Biophysical Journal, 2003, 85, 2641-2649.	0.2	58
162	Ab InitioMolecular Dynamics for Molecules with Variable Numbers of Electrons. Physical Review Letters, 2002, 88, 213002.	2.9	82

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163	The interplay between protein dynamics and frustration of non-bonded interactions as revealed by molecular dynamics simulations. Chemical Physics Letters, 2001, 345, 287-294.	1.2	10
164	Dynamic properties of monomeric insect erythrocruorin III from Chironomus thummi-thummi: relationships between structural flexibility and functional complexity. Biophysical Journal, 1997, 73, 2742-2751.	0.2	8
165	Algorithmic Error Mitigation Scheme for Current Quantum Processors. Quantum - the Open Journal for Quantum Science, 0, 5, 492.	0.0	24
166	Improving Variational Quantum Optimization using CVaR. Quantum - the Open Journal for Quantum Science, 0, 4, 256.	0.0	94
167	Improving readout in quantum simulations with repetition codes. Quantum Science and Technology, 0, , .	2.6	9