Nadia Rega

List of Publications by Year in descending order

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92 papers	12,584 citations	134610 34 h-index	54771 88 g-index
94 all docs	94 docs citations	94 times ranked	14431 citing authors

#	Article	IF	Citations
1	Free Energy Profiles of Proton Transfer Reactions: Density Functional Benchmark from Biased Ab Initio Dynamics. Journal of Chemical Theory and Computation, 2022, , .	2.3	5
2	Ultrafast photo-induced processes in complex environments: The role of accuracy in excited-state energy potentials and initial conditions. Chemical Physics Reviews, 2022, 3, .	2.6	7
3	Direct observation of the solvent organization and nuclear vibrations of [Ru(dcbpy)₂(NCS)₂]^{4â^'}, [dcbpy = (4,4â€²-dicarboxy-2,2â€²-bipyridine)], via ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2021, 23, 22885-22896.	1.3	12
4	Water-Mediated Excited State Proton Transfer of Pyranineâ€“Acetate in Aqueous Solution: Vibrational Fingerprints from Ab Initio Molecular Dynamics. Journal of Physical Chemistry A, 2021, 125, 3569-3578.	1.1	11
5	Interference of Polydatin/Resveratrol in the ACE2:Spike Recognition during COVID-19 Infection. A Focus on Their Potential Mechanism of Action through Computational and Biochemical Assays. Biomolecules, 2021, 11, 1048.	1.8	22
6	Structural Origin and Vibrational Fingerprints of the Ultrafast Excited State Proton Transfer of the Pyranine-Acetate Complex in Aqueous Solution. Journal of Physical Chemistry B, 2021, 125, 10273-10281.	1.2	8
7	Exploring the Franckâ€“Condon region of a photoexcited charge transfer complex in solution to interpret femtosecond stimulated Raman spectroscopy: excited state electronic structure methods to unveil non-radiative pathways. Chemical Science, 2021, 12, 8058-8072.	3.7	14
8	Shedding light on the interaction of polydatin and resveratrol with G-quadruplex and duplex DNA: a biophysical, computational and biological approach. International Journal of Biological Macromolecules, 2020, 151, 1163-1172.	3.6	27
9	Time-Resolved Vibrational Analysis of Excited State Ab Initio Molecular Dynamics to Understand Photorelaxation: The Case of the Pyranine Photoacid in Aqueous Solution. Journal of Chemical Theory and Computation, 2020, 16, 6007-6013.	2.3	23
10	A Not Obvious Correlation Between the Structure of Green Fluorescent Protein Chromophore Pocket and Hydrogen Bond Dynamics: A Choreography From ab initio Molecular Dynamics. Frontiers in Molecular Biosciences, 2020, 7, 569990.	1.6	23
11	Abâ€initio molecular dynamics and hybrid explicitâ€implicit solvation model for aqueous and nonaqueous solvents: <scp>GFP</scp> chromophore in water and methanol solution as case study. Journal of Computational Chemistry, 2020, 41, 2228-2239.	1.5	27
12	Modeling the Electron Transfer Chain in an Artificial Photosynthetic Machine. Journal of Physical Chemistry Letters, 2020, 11, 9738-9744.	2.1	0
13	Modeling Excited-State Proton Transfer to Solvent: A Dynamics Study of a Super Photoacid with a Hybrid Implicit/Explicit Solvent Model. Journal of Chemical Theory and Computation, 2020, 16, 7033-7043.	2.3	26
14	Cover Image, Volume 41, Issue 26. Journal of Computational Chemistry, 2020, 41, C2.	1.5	0
15	Multiresolution continuous wavelet transform for studying coupled soluteâ€“solvent vibrations via ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2020, 22, 22645-22661.	1.3	26
16	An electron density based analysis to establish the electronic adiabaticity of proton coupled electron transfer reactions. Journal of Computational Chemistry, 2020, 41, 1835-1841.	1.5	11
17	Unveiling anharmonic coupling by means of excited state ab initio dynamics: application to diarylethene photoreactivity. Physical Chemistry Chemical Physics, 2019, 21, 3606-3614.	1.3	28
18	Iron(III) Complexes for Highly Efficient and Sustainable Ketalization of Glycerol: A Combined Experimental and Theoretical Study. ACS Omega, 2019, 4, 688-698.	1.6	43

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19	Exploring Nuclear Photorelaxation of Pyranine in Aqueous Solution: an Integrated Ab-Initio Molecular Dynamics and Time Resolved Vibrational Analysis Approach. Journal of Physical Chemistry A, 2018, 122, 2884-2893.	1.1	29
20	Turn-on fluorescence detection of protein by molecularly imprinted hydrogels based on supramolecular assembly of peptide multi-functional blocks. Journal of Materials Chemistry B, 2018, 6, 1207-1215.	2.9	31
21	The mechanism of a green fluorescent protein proton shuttle unveiled in the time-resolved frequency domain by excited state ab initio dynamics. Chemical Science, 2018, 9, 1126-1135.	3.7	43
22	Unveiling the structure of a novel artificial hemeâ€enzyme with peroxidaseâ€like activity: A theoretical investigation. Biopolymers, 2018, 109, e23225.	1.2	14
23	Comparing the performance of TDâ€DFT and SACâ€CI methods in the description of excited states potential energy surfaces: An excited state proton transfer reaction as case study. Journal of Computational Chemistry, 2017, 38, 1084-1092.	1.5	15
24	Excitedâ€State Proton Transfer and Intramolecular Charge Transfer in 1,3â€Diketone Molecules. ChemPhysChem, 2016, 17, 1530-1538.	1.0	12
25	On the different strength of photoacids. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	25
26	A qualitative model to identify non-radiative decay channels: the spiropyran as case study. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	15
27	â€œWatchingâ€•Polaron Pair Formation from First-Principles Electronâ€“Nuclear Dynamics. Journal of Physical Chemistry A, 2016, 120, 7255-7261.	1.1	47
28	On the Driving Force of the Excited-State Proton Shuttle in the Green Fluorescent Protein: A Time-Dependent Density Functional Theory (TD-DFT) Study of the Intrinsic Reaction Path. Journal of Chemical Theory and Computation, 2016, 12, 4925-4933.	2.3	33
29	Unveiling the Reactivity of a Synthetic Mimic of the Oxygen Evolving Complex. Journal of Physical Chemistry Letters, 2016, 7, 5015-5021.	2.1	16
30	Electronic spectroscopy of a solvatochromic dye in water: comparison of static cluster/implicit and dynamical/explicit solvent models on structures and energies. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	7
31	Intrinsic and Dynamical Reaction Pathways of an Excited State Proton Transfer. Journal of Physical Chemistry B, 2015, 119, 2650-2657.	1.2	32
32	Exploring excited states using Time Dependent Density Functional Theory and density-based indexes. Coordination Chemistry Reviews, 2015, 304-305, 166-178.	9.5	118
33	Absorption and Emission Spectral Shapes of a Prototype Dye in Water by Combining Classical/Dynamical and Quantum/Static Approaches. Journal of Physical Chemistry A, 2015, 119, 5426-5438.	1.1	50
34	Describing Excited State Intramolecular Proton Transfer in Dual Emissive Systems: A Density Functional Theory Based Analysis. Journal of Physical Chemistry B, 2015, 119, 2459-2466.	1.2	38
35	Understanding THz and IR Signals beneath Time-Resolved Fluorescence from Excited-State Ab Initio Dynamics. Journal of the American Chemical Society, 2014, 136, 14866-14874.	6.6	41
36	Integration of binding peptide selection and multifunctional particles as tool-box for capture of soluble proteins in serum. Journal of the Royal Society Interface, 2014, 11, 20140718.	1.5	15

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37	Intermolecular proton shuttling in excited state proton transfer reactions: insights from theory. Physical Chemistry Chemical Physics, 2014, 16, 8661-8666.	1.3	34
38	Non-radiative decay paths in rhodamines: new theoretical insights. Physical Chemistry Chemical Physics, 2014, 16, 20681-20688.	1.3	44
39	Modeling of charge transfer processes to understand photophysical signatures: The case of Rhodamine 110. Chemical Physics Letters, 2014, 610-611, 148-152.	1.2	17
40	From charge-transfer to a charge-separated state: a perspective from the real-time TDDFT excitonic dynamics. Physical Chemistry Chemical Physics, 2014, 16, 24457-24465.	1.3	51
41	On the optical absorption of the anionic GFP chromophore in vacuum, solution, and protein. Physical Chemistry Chemical Physics, 2013, 15, 20536.	1.3	41
42	Exploring the Metric of Excited State Proton Transfer Reactions. Journal of Physical Chemistry B, 2013, 117, 16165-16173.	1.2	51
43	Effects of molecular dynamics and solvation on the electronic structure of molecular probes. Highlights in Theoretical Chemistry, 2013, , 339-350.	0.0	0
44	Fluorescence Lifetimes and Quantum Yields of Rhodamine Derivatives: New Insights from Theory and Experiment. Journal of Physical Chemistry A, 2012, 116, 7491-7497.	1.1	108
45	Effects of molecular dynamics and solvation on the electronic structure of molecular probes. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	5
46	Preface to the special collection in honour of Vincenzo Barone. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	0
47	Methyl Phosphate Dianion Hydrolysis in Solution Characterized by Path Collective Variables Coupled with DFT-Based Enhanced Sampling Simulations. Journal of Chemical Theory and Computation, 2011, 7, 539-543.	2.3	36
48	Vibrational analysis of x-ray absorption fine structure thermal factors by ab initio molecular dynamics: The Zn(II) ion in aqueous solution as a case study. Journal of Chemical Physics, 2011, 134, 074504.	1.2	29
49	Microsolvation of uracil anion radical in aqueous solution: a QM/MM study. Chemical Physics Letters, 2010, 500, 104-110.	1.2	7
50	Magnetic Properties of Nitroxide Spin Probes: Reliable Account of Molecular Motions and Nonspecific Solvent Effects by Time-Dependent and Time-Independent Approaches. Journal of Physical Chemistry B, 2010, 114, 11509-11514.	1.2	25
51	Uracil anion radical in aqueous solution: thermodynamics versus spectroscopy. Physical Chemistry Chemical Physics, 2010, 12, 10736.	1.3	9
52	Molecular dynamics simulations in a NpT ensemble using non-periodic boundary conditions. Chemical Physics Letters, 2009, 483, 177-181.	1.2	16
53	Theoretical modeling of open-shell molecules in solution: a QM/MM molecular dynamics approach. Theoretical Chemistry Accounts, 2008, 120, 499-506.	0.5	7
54	Microsolvation of the Zn(II) ion in aqueous solution: A hybrid QM/MM MD approach using non-periodic boundary conditions. Chemical Physics Letters, 2008, 451, 53-57.	1.2	20

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55	Implementation and validation of DFT-D for molecular vibrations and dynamics: The benzene dimer as a case study. Chemical Physics Letters, 2008, 452, 333-339.	1.2	46
56	A discrete/continuum QM/MM MD study of the triplet state of acetone in aqueous solution. Chemical Physics Letters, 2008, 453, 202-206.	1.2	12
57	Quantum Mechanical Computations and Spectroscopy: From Small Rigid Molecules in the Gas Phase to Large Flexible Molecules in Solution. Accounts of Chemical Research, 2008, 41, 605-616.	7.6	155
58	A hybrid explicit/implicit solvation method for first-principle molecular dynamics simulations. Journal of Chemical Physics, 2008, 128, 144501.	1.2	79
59	Accurate Density Functional Calculations of Near-Edge X-Ray and Optical Absorption Spectra of Liquid Water Using Nonperiodic Boundary Conditions: The Role of Self-Interaction and Long-Range Effects. Physical Review Letters, 2008, 100, 107401.	2.9	43
60	Unraveling the Role of Stereo-electronic, Dynamical, and Environmental Effects in Tuning the Structure and Magnetic Properties of Glycine Radical in Aqueous Solution at Different pH Values. Journal of the American Chemical Society, 2007, 129, 15380-15390.	6.6	40
61	Theoretical modeling of spectroscopic properties of molecules in solution: toward an effective dynamical discrete/continuum approach. Theoretical Chemistry Accounts, 2007, 117, 1001-1015.	0.5	59
62	Non-periodic boundary conditions for ab initio molecular dynamics in condensed phase using localized basis functions. Chemical Physics Letters, 2006, 422, 367-371.	1.2	54
63	Vibrational Analysis Beyond the Harmonic Regime From Ab-initio Molecular Dynamics. Theoretical Chemistry Accounts, 2006, 116, 347-354.	0.5	29
64	Solvent Effects on the UV (n â†' Ï€*) and NMR (17O) Spectra of Acetone in Aqueous Solution: Development and Validation of a Modified AMBER Force Field for an Integrated MD/DFT/PCM Approach. Theoretical Chemistry Accounts, 2006, 116, 456-461.	0.5	18
65	A polarizable continuum approach for the study of heterogeneous dielectric environments. Journal of Chemical Physics, 2006, 124, 184103.	1.2	17
66	Reliable molecular simulations of solute-solvent systems with a minimum number of solvent shells. Journal of Chemical Physics, 2006, 124, 214505.	1.2	39
67	A quantum mechanical/molecular dynamics/mean field study of acrolein in aqueous solution: Analysis of H bonding and bulk effects on spectroscopic properties. Journal of Chemical Physics, 2006, 125, 164515.	1.2	65
68	Vibrational computations beyond the harmonic approximation: Performances of the B3LYP density functional for semirigid molecules. Journal of Computational Chemistry, 2005, 26, 384-388.	1.5	179
69	A computational protocol to probe the role of solvation effects on the reduction potential of azurin mutants. Proteins: Structure, Function and Bioinformatics, 2005, 62, 262-269.	1.5	10
70	Understanding Electron Transfer across Negatively-Charged Aib Oligopeptides. Journal of Physical Chemistry B, 2005, 109, 1023-1033.	1.2	31
71	Computation of protein pKâ€™s values by an integrated density functional theory/Polarizable Continuum Model approach. Theoretical Chemistry Accounts, 2004, 111, 237-245.	0.5	54
72	Accurate vibrational spectra of large molecules by density functional computations beyond the harmonic approximation: the case of uracil and 2-thiouracil. Chemical Physics Letters, 2004, 388, 279-283.	1.2	104

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73	Hybrid Ab-Initio/Empirical Molecular Dynamics:â€‰Combining the ONIOM Scheme with the Atom-Centered Density Matrix Propagation (ADMP) Approach. Journal of Physical Chemistry B, 2004, 108, 4210-4220.	1.2	131
74	Energies, structures, and electronic properties of molecules in solution with the C-PCM solvation model. Journal of Computational Chemistry, 2003, 24, 669-681.	1.5	6,758
75	New developments in the polarizable continuum model for quantum mechanical and classical calculations on molecules in solution. Journal of Chemical Physics, 2002, 117, 43-54.	1.2	2,235
76	Finite Elements Molecular Surfaces in Continuum Solvent Models for Large Chemical Systems. Journal of Computational Methods in Sciences and Engineering, 2002, 2, 469-474.	0.1	8
77	Conformational analysis of the tyrosine dipeptide analogue in the gas phase and in aqueous solution by a density functional/continuum solvent model. Journal of Computational Chemistry, 2002, 23, 650-661.	1.5	32
78	Interplay of Intrinsic and Environmental Effects on the Magnetic Properties of Free Radicals Issuing from H-Atom Addition to Cytosine. Journal of the American Chemical Society, 2001, 123, 7113-7117.	6.6	22
79	Conformational Behavior of Macromolecules in Solution. Homopolypeptides of Î±-Aminoisobutyric Acid as Test Cases. Macromolecules, 2001, 34, 7550-7557.	2.2	30
80	New computational strategies for the quantum mechanical study of biological systems in condensed phases. Theoretical and Computational Chemistry, 2001, , 467-538.	0.2	18
81	Polarizable dielectric model of solvation with inclusion of charge penetration effects. Journal of Chemical Physics, 2001, 114, 5691-5701.	1.2	315
82	A plane wave implementation of the polarizable continuum model. Chemical Physics Letters, 2000, 328, 302-309.	1.2	11
83	Quantum Mechanical Conformational Analysis of Î²-Alanine Zwitterion in Aqueous Solution. Journal of the American Chemical Society, 2000, 122, 3151-3155.	6.6	39
84	Medium-dependent competitive pathways in the reactions of polyunsaturated fatty acids with nitric oxide in the presence of oxygen. Structural characterisation of nitration products and a theoretical insight. Tetrahedron, 1999, 55, 9297-9308.	1.0	21
85	Toward an effective and reliable representation of solvent effects in the study of biochemical systems. International Journal of Quantum Chemistry, 1999, 73, 219-227.	1.0	12
86	Improving performance of polarizable continuum model for study of large molecules in solution. Journal of Computational Chemistry, 1999, 20, 1186-1198.	1.5	25
87	Ring-Opening Reaction of Cyclobutene Radical Cation: Effect of Solvent on Competing Pathways. Journal of Physical Chemistry A, 1999, 103, 217-219.	1.1	19
88	Towards linear scaling in continuum solvent models.. Chemical Physics Letters, 1998, 293, 221-229.	1.2	34
89	Structures and Spectroscopic Characteristics of 5,6-Dihydro-6-thymyl and 5,6-Dihydro-5-thymyl Radicals by an Integrated Quantum Mechanical Approach Including Electronic, Vibrational, and Solvent Effects. Journal of the American Chemical Society, 1998, 120, 1864-1871.	6.6	60
90	Structure and Magnetic Properties of Glycine Radical in Aqueous Solution at Different pH Values. Journal of the American Chemical Society, 1998, 120, 5723-5732.	6.6	88

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91	Intrinsic and Environmental Effects in the Structure and Magnetic Properties of Glycine Radical in Aqueous Solution. Journal of the American Chemical Society, 1997, 119, 12962-12967.	6.6	87
92	Development and validation of reliable quantum mechanical approaches for the study of free radicals in solution. Journal of Chemical Physics, 1996, 105, 11060-11067.	1.2	206