Alessio Petrone

List of Publications by Year
in descending order

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Version: 2024-02-01

37 papers	1,493 citations	279798 23 h-index	361022 35 g-index
37 all docs	37 docs citations	37 times ranked	2200 citing authors

#	Article	IF	Citations
1	Ultrafast photo-induced processes in complex environments: The role of accuracy in excited-state energy potentials and initial conditions. Chemical Physics Reviews, 2022, 3, .	5.7	7
2	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.	2.8	12
3	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.	4.0	22
4	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.	7.4	14
5	The Chronus Quantum software package. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1436.	14.6	66
6	Spectroscopic Signatures of the B and H₄ Polyatomic Nitrogen Aggregates in Nanodiamond. Journal of Physical Chemistry C, 2020, 124, 18275-18283.	3.1	5
7	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.	3.5	23
8	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.	3.3	27
9	Cover Image, Volume 41, Issue 26. Journal of Computational Chemistry, 2020, 41, C2.	3.3	0
10	Multiresolution continuous wavelet transform for studying coupled soluteâ€“solvent vibrations via ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2020, 22, 22645-22661.	2.8	26
11	High-pressure, high-temperature molecular doping of nanodiamond. Science Advances, 2019, 5, eaau6073.	10.3	40
12	Carboxylate Anchors Act as Exciton Reporters in 1.3 nm Indium Phosphide Nanoclusters. Journal of Physical Chemistry Letters, 2019, 10, 1833-1839.	4.6	23
13	Effect of Surface Passivation on Nanodiamond Crystallinity. Journal of Physical Chemistry C, 2018, 122, 8573-8580.	3.1	24
14	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.	7.4	43
15	Efficient Implementation of Variation after Projection Generalized Hartreeâ€“Fock. Journal of Chemical Theory and Computation, 2018, 14, 588-596.	5.3	14
16	Electronic structures and spectroscopic signatures of silicon-vacancy containing nanodiamonds. Physical Review B, 2018, 98, .	3.2	16
17	Mapping Vibronic Couplings in a Solar Cell Dye with Polarization-Selective Two-Dimensional Electronicâ€“Vibrational Spectroscopy. Journal of Physical Chemistry Letters, 2018, 9, 6289-6295.	4.6	31
18	An efficient implementation of two-component relativistic density functional theory with torque-free auxiliary variables. European Physical Journal B, 2018, 91, 1.	1.5	54

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19	Ab Initio Excited-State Transient Raman Analysis. Journal of Physical Chemistry A, 2017, 121, 3958-3965.	2.5	16
20	Investigating the role of amine in InP nanocrystal synthesis: destabilizing cluster intermediates by Z-type ligand displacement. Chemical Communications, 2017, 53, 161-164.	4.1	55
21	Cation Exchange Induced Transformation of InP Magic-Sized Clusters. Chemistry of Materials, 2017, 29, 7984-7992.	6.7	67
22	Mixed Cation FA_xPEA_{1â€“}_xPbI₃ with Enhanced Phase and Ambient Stability toward Highâ€Performance Perovskite Solar Cells. Advanced Energy Materials, 2017, 7, 1601307.	19.5	298
23	Does Thermal Breathing Affect Collision Cross Sections of Gas-Phase Peptide Ions? An Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry Letters, 2016, 7, 2765-2771.	4.6	16
24	Quantum confinement effects on optical transitions in nanodiamonds containing nitrogen vacancies. Physical Review B, 2016, 94, .	3.2	36
25	â€œWatchingâ€•Polaron Pair Formation from First-Principles Electronâ€“Nuclear Dynamics. Journal of Physical Chemistry A, 2016, 120, 7255-7261.	2.5	47
26	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.	5.3	33
27	Classical or Quantum? A Computational Study of Small Ion Diffusion in IIâ€“VI Semiconductor Quantum Dots. Journal of Physical Chemistry C, 2016, 120, 19434-19441.	3.1	16
28	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.	1.4	7
29	Ab Initio Transient Vibrational Spectral Analysis. Journal of Physical Chemistry Letters, 2016, 7, 4501-4508.	4.6	37
30	Single-Crystal and Electronic Structure of a 1.3 nm Indium Phosphide Nanocluster. Journal of the American Chemical Society, 2016, 138, 1510-1513.	13.7	164
31	Direct ab Initio (Meta-)Surface-Hopping Dynamics. Journal of Chemical Theory and Computation, 2016, 12, 935-945.	5.3	40
32	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.	2.5	50
33	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.	13.7	41
34	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.	2.8	51
35	On the optical absorption of the anionic GFP chromophore in vacuum, solution, and protein. Physical Chemistry Chemical Physics, 2013, 15, 20536.	2.8	41
36	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.	3.0	29

#	Article	IF	Citations
37	Switchable light vs acid-induced transformations of complex framework compounds at room temperature. Green Chemistry, 0, , .	9.0	2