Alessio Petrone

List of Publications by Year
in descending order

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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	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
2	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
3	Cation Exchange Induced Transformation of InP Magic-Sized Clusters. Chemistry of Materials, 2017, 29, 7984-7992.	6.7	67
4	The Chronus Quantum software package. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1436.	14.6	66
5	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
6	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
7	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
8	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
9	â€œWatchingâ€•Polaron Pair Formation from First-Principles Electronâ€“Nuclear Dynamics. Journal of Physical Chemistry A, 2016, 120, 7255-7261.	2.5	47
10	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
11	On the optical absorption of the anionic GFP chromophore in vacuum, solution, and protein. Physical Chemistry Chemical Physics, 2013, 15, 20536.	2.8	41
12	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
13	Direct ab Initio (Meta-)Surface-Hopping Dynamics. Journal of Chemical Theory and Computation, 2016, 12, 935-945.	5.3	40
14	High-pressure, high-temperature molecular doping of nanodiamond. Science Advances, 2019, 5, eaau6073.	10.3	40
15	Ab Initio Transient Vibrational Spectral Analysis. Journal of Physical Chemistry Letters, 2016, 7, 4501-4508.	4.6	37
16	Quantum confinement effects on optical transitions in nanodiamonds containing nitrogen vacancies. Physical Review B, 2016, 94, .	3.2	36
17	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
18	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

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19	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
20	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
21	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
22	Effect of Surface Passivation on Nanodiamond Crystallinity. Journal of Physical Chemistry C, 2018, 122, 8573-8580.	3.1	24
23	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
24	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
25	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
26	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
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	Ab Initio Excited-State Transient Raman Analysis. Journal of Physical Chemistry A, 2017, 121, 3958-3965.	2.5	16
29	Electronic structures and spectroscopic signatures of silicon-vacancy containing nanodiamonds. Physical Review B, 2018, 98, .	3.2	16
30	Efficient Implementation of Variation after Projection Generalized Hartreeâ€“Fock. Journal of Chemical Theory and Computation, 2018, 14, 588-596.	5.3	14
31	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
32	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
33	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
34	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
35	Spectroscopic Signatures of the B and H₄ Polyatomic Nitrogen Aggregates in Nanodiamond. Journal of Physical Chemistry C, 2020, 124, 18275-18283.	3.1	5
36	Switchable light vs acid-induced transformations of complex framework compounds at room temperature. Green Chemistry, 0, , .	9.0	2

#	Article	IF	Citations
37	Cover Image, Volume 41, Issue 26. Journal of Computational Chemistry, 2020, 41, C2.	3.3	0