Francesco Buda

List of Publications by Year
in descending order

58	2,137	279798	233421
papers	citations	23 h-index	45 g-index

60	60	60	2776
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Analytical Nonadiabatic Couplings and Gradients within the State-Averaged Orbital-Optimized Variational Quantum Eigensolver. Journal of Chemical Theory and Computation, 2022, 18, 776-794.	5.3	14
2	The role of chirality and plastic crystallinity in the optical and mechanical properties of chlorosomes. IScience, 2022, 25, 103618.	4.1	3
3	Freestanding non-covalent thin films of the propeller-shaped polycyclic aromatic hydrocarbon decacyclene. Nature Communications, 2022, 13, 1920.	12.8	1
4	Tuning the Protonâ€Coupled Electronâ€Transfer Rate by Ligand Modification in Catalystâ€“Dye Supramolecular Complexes for Photocatalytic Water Splitting. ChemSusChem, 2021, 14, 479-486.	6.8	7
5	A state-averaged orbital-optimized hybrid quantumâ€“classical algorithm for a democratic description of ground and excited states. Quantum Science and Technology, 2021, 6, 024004.	5.8	38
6	Twoâ€Channel Model for Electron Transfer in a Dyeâ€Catalystâ€Dye Supramolecular Complex for Photocatalytic Water Splitting. ChemSusChem, 2021, 14, 3155-3162.	6.8	8
7	Efficient workflow for the investigation of the catalytic cycle of water oxidation catalysts: Combining <scp>GFNâ€xTB</scp> and density functional theory. Journal of Computational Chemistry, 2021, 42, 1885-1894.	3.3	11
8	Orbital transformations to reduce the 1-norm of the electronic structure Hamiltonian for quantum computing applications. Physical Review Research, 2021, 3, .	3.6	19
9	Intracellular Dynamic Assembly of Deepâ€Red Emitting Supramolecular Nanostructures Based on the Ptâ¦Pt Metallophilic Interaction. Advanced Materials, 2021, 33, e2008613.	21.0	17
10	Automated assessment of redox potentials for dyes in dye-sensitized photoelectrochemical cells. Physical Chemistry Chemical Physics, 2021, 24, 197-210.	2.8	4
11	Systematic Computational Design and Optimization of Light Absorbing Dyes. Journal of Physical Chemistry A, 2020, 124, 6380-6388.	2.5	10
12	Photoinduced Electron Injection in a Fully Solvated Dye-Sensitized Photoanode: A Dynamical Semiempirical Study. Journal of Physical Chemistry C, 2020, 124, 27965-27976.	3.1	11
13	Dynamic Disorder Drives Exciton Transfer in Tubular Chlorosomal Assemblies. Journal of Physical Chemistry B, 2020, 124, 4026-4035.	2.6	16
14	Power generation by reverse electrodialysis in a single-layer nanoporous membrane made from coreâ€“rim polycyclic aromatic hydrocarbons. Nature Nanotechnology, 2020, 15, 307-312.	31.5	127
15	Photocatalytic Water Splitting Cycle in a Dye-Catalyst Supramolecular Complex: Ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2019, 123, 21403-21414.	3.1	17
16	Photoinduced Electron Transfer in Donorâ€“Acceptor Complexes: Isotope Effect and Dynamic Symmetry Breaking. Journal of Physical Chemistry Letters, 2019, 10, 6504-6511.	4.6	12
17	Molecular Insight in the Optical Response of Tubular Chlorosomal Assemblies. Journal of Physical Chemistry C, 2019, 123, 16462-16478.	3.1	13
18	Calculating energy derivatives for quantum chemistry on a quantum computer. Npj Quantum Information, 2019, 5, .	6.7	55

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19	Proton Acceptor near the Active Site Lowers Dramatically the Oâ€“O Bond Formation Energy Barrier in Photocatalytic Water Splitting. Journal of Physical Chemistry Letters, 2019, 10, 7690-7697.	4.6	13
20	The Dynamic Origin of Color Tuning in Proteins Revealed by a Carotenoid Pigment. Journal of Physical Chemistry Letters, 2018, 9, 2404-2410.	4.6	26
21	Contrasting Modes of Self-Assembly and Hydrogen-Bonding Heterogeneity in Chlorosomes of Chlorobaculum tepidum. Journal of Physical Chemistry C, 2018, 122, 14877-14888.	3.1	20
22	Energetic Effects of a Closed System Approach Including Explicit Proton and Electron Acceptors as Demonstrated by a Mononuclear Ruthenium Water Oxidation Catalyst. ChemCatChem, 2018, 10, 4594-4601.	3.7	6
23	Pathways to electrochemical solar-hydrogen technologies. Energy and Environmental Science, 2018, 11, 2768-2783.	30.8	238
24	A Quantumâ€mechanical Study of the Binding Pocket of Proteorhodopsin: Absorption and Vibrational Spectra Modulated by Analogue Chromophores. Photochemistry and Photobiology, 2017, 93, 1399-1406.	2.5	7
25	Introducing a closed system approach for the investigation of chemical steps involving proton and electron transfer; as illustrated by a copper-based water oxidation catalyst. Physical Chemistry Chemical Physics, 2017, 19, 4208-4215.	2.8	13
26	A Dynamic View of Proton-Coupled Electron Transfer in Photocatalytic Water Splitting. Journal of Physical Chemistry C, 2016, 120, 23074-23082.	3.1	23
27	Crucial Role of Nuclear Dynamics for Electron Injection in a Dyeâ€“Semiconductor Complex. Journal of Physical Chemistry Letters, 2015, 6, 2393-2398.	4.6	49
28	Realâ€time Simulations of Photoinduced Coherent Charge Transfer and Protonâ€Coupled Electron Transfer. ChemPhysChem, 2014, 15, 3258-3263.	2.1	10
29	In-Silico Design of a Donorâ€“Antennaâ€“Acceptor Supramolecular Complex for Photoinduced Charge Separation. Journal of Physical Chemistry C, 2014, 118, 15600-15609.	3.1	23
30	Molecular Catalytic Assemblies for Electrodriven Water Splitting. ChemPlusChem, 2013, 78, 35-47.	2.8	47
31	Solid-State NMR of Nanomachines Involved in Photosynthetic Energy Conversion. Annual Review of Biophysics, 2013, 42, 675-699.	10.0	12
32	Proton Displacements Coupled to Primary Electron Transfer in the Rhodobacter sphaeroides Reaction Center. Journal of Physical Chemistry B, 2013, 117, 11162-11168.	2.6	25
33	Bathochromic Shift in Green Fluorescent Protein: A Puzzle for QM/MM Approaches. Journal of Chemical Theory and Computation, 2012, 8, 112-124.	5.3	94
34	Mechanism and Reaction Coordinate of Directional Charge Separation in Bacterial Reaction Centers. Journal of Physical Chemistry Letters, 2012, 3, 694-697.	4.6	42
35	Ab Initio Molecular Dynamics Study of Water Oxidation Reaction Pathways in Monoâ€Ru Catalysts. ChemPhysChem, 2012, 13, 140-146.	2.1	45
36	Theoretical Spectroscopy of Astaxanthin in Crustacyanin Proteins: Absorption, Circular Dichroism, and Nuclear Magnetic Resonance. Journal of Physical Chemistry B, 2011, 115, 3216-3225.	2.6	33

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37	Zinc chlorins for artificial light-harvesting self-assemble into antiparallel stacks forming a microcrystalline solid-state material. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 11472-11477.	7.1	67
38	Alternating syn-anti bacteriochlorophylls form concentric helical nanotubes in chlorosomes. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 8525-8530.	7.1	283
39	Introduction to theory/modeling methods in photosynthesis. Photosynthesis Research, 2009, 102, 437-441.	2.9	8
40	Differential Charge Polarization of Axial Histidines in Bacterial Reaction Centers Balances the Asymmetry of the Special Pair. Journal of the American Chemical Society, 2009, 131, 9626-9627.	13.7	20
41	Absorption Spectrum of the Green Fluorescent Protein Chromophore: A Difficult Case for ab Initio Methods?. Journal of Chemical Theory and Computation, 2009, 5, 2074-2087.	5.3	134
42	Protein-induced geometric constraints and charge transfer in bacteriochlorophyllâ€“histidine complexes in LH2. Physical Chemistry Chemical Physics, 2008, 10, 6971.	2.8	19
43	Density Functional Theory and Car-Parrinello Molecular Dynamics Methods. Advances in Photosynthesis and Respiration, 2008, , 487-499.	1.0	1
44	Mechanism of Bleomycin Suicide:Â A Carâ^'Parrinello Molecular Dynamics Investigation. Journal of Physical Chemistry B, 2006, 110, 21245-21250.	2.6	2
45	Crystallographic evidence of theoretically novel anionâ€“Ï€ interactions. New Journal of Chemistry, 2006, 30, 1561-1566.	2.8	55
46	Carâ€“Parrinello Molecular Dynamics Study of the Blue-Shifted F3CHâ‹…â‹…â‹…FCD3 System in Liquid N2. ChemPhysChem, 2006, 7, 1221-1228.	2.1	12
47	Trigonal-Prismatic vs. Octahedral Geometry for MnII Complexes with Innocent Didentate Ligands: A Subtle Difference as Shown by XRD and DFT on [Mn(acac)2(bpy)]. European Journal of Inorganic Chemistry, 2005, 2005, 2255-2261.	2.0	47
48	Car-Parrinello Molecular Dynamics Study of a Blue-Shifted Intermolecular Weak-Hydrogen-Bond System. ChemPhysChem, 2005, 6, 1719-1724.	2.1	14
49	The metal bonding domain of the antitumor drug Fe(II)-bleomycin: a DFT investigation. Journal of Biological Inorganic Chemistry, 2005, 10, 33-40.	2.6	10
50	Spectroscopy and Quantum Chemical Modeling Reveal a Predominant Contribution of Excitonic Interactions to the Bathochromic Shift in Î±-Crustacyanin, the Blue Carotenoprotein in the Carapace of the LobsterHomarus gammarus. Journal of the American Chemical Society, 2005, 127, 1438-1445.	13.7	50
51	DFT calculations of the 1H chemical shifts and 13C chemical shift tensors of retinal isomers. Computational and Theoretical Chemistry, 2004, 711, 141-147.	1.5	9
52	Methane-to-Methanol Oxidation by the Hydrated Iron(IV) Oxo Species in Aqueous Solution:Â A Combined DFT and Carâ^'Parrinello Molecular Dynamics Study. Journal of the American Chemical Society, 2004, 126, 4355-4365.	13.7	102
53	Fullerene-like IIIâ^'V Clusters:Â A Density Functional Theory Prediction. Journal of Physical Chemistry B, 2001, 105, 12477-12480.	2.6	34
54	The transition state in the isomerization of rhodopsin. Chemical Physics Letters, 1998, 294, 447-453.	2.6	35

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55	Ab initio molecular dynamics of rhodopsin. Pure and Applied Chemistry, 1997, 69, 2105-2110.	1.9	21
56	Energy Storage in the Primary Photoproduct of Vision. Journal of Physical Chemistry B, 1997, 101, 2954-2958.	2.6	55
57	Charge Localization and Dynamics in Rhodopsin. Physical Review Letters, 1996, 77, 4474-4477.	7.8	47
58	In Silico Optimization of Charge Separating Dyes for Solar Energy Conversion. ChemSusChem, 0, , .	6.8	3