Alberto Fabrizio

List of Publications by Year
in descending order

25	853	686830 13	610482 24
papers	citations	h-index	g-index

27	27	27	1345
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	SPA^HM: the spectrum of approximated Hamiltonian matrices representations. , 2022, 1, 286-294.		7
2	Local Kernel Regression and Neural Network Approaches to the Conformational Landscapes of Oligopeptides. Journal of Chemical Theory and Computation, 2022, 18, 1467-1479.	2.3	8
3	Learning the Exciton Properties of Azo-dyes. Journal of Physical Chemistry Letters, 2021, 12, 5957-5962.	2.1	4
4	Impact of quantum-chemical metrics on the machine learning prediction of electron density. Journal of Chemical Physics, 2021, 155, 024107.	1.2	3
5	Data-powered augmented volcano plots for homogeneous catalysis. Chemical Science, 2020, 11, 12070-12080.	3.7	23
6	Learning (from) the Electron Density: Transferability, Conformational and Chemical Diversity. Chimia, 2020, 74, 232-236.	0.3	9
7	Machine learning models of the energy curvature vs particle number for optimal tuning of long-range corrected functionals. Journal of Chemical Physics, 2020, 152, 154103.	1.2	12
8	Hamiltonian-Reservoir Replica Exchange and Machine Learning Potentials for Computational Organic Chemistry. Journal of Chemical Theory and Computation, 2020, 16, 3084-3094.	2.3	16
9	Balancing Density Functional Theory Interaction Energies in Charged Dimers Precursors to Organic Semiconductors. Journal of Chemical Theory and Computation, 2020, 16, 3530-3542.	2.3	2
10	Learning on-top: Regressing the on-top pair density for real-space visualization of electron correlation. Journal of Chemical Physics, 2020, 153, 204111.	1.2	10
11	Tuning the structure, reactivity and magnetic communication of nitride-bridged uranium complexes with the ancillary ligands. Chemical Science, 2019, 10, 8840-8849.	3.7	26
12	Open-Shell Nonbenzenoid Nanographenes Containing Two Pairs of Pentagonal and Heptagonal Rings. Journal of the American Chemical Society, 2019, 141, 12011-12020.	6.6	112
13	Electron density learning of non-covalent systems. Chemical Science, 2019, 10, 9424-9432.	3.7	92
14	Synthesis of aminyl biradicals by base-induced Csp³â€“Csp³ coupling of cationic azo dyes. Chemical Science, 2019, 10, 5719-5724.	3.7	30
15	Data Mining the Câ^'C Crossâ€Coupling Genome. ChemCatChem, 2019, 11, 4096-4107.	1.8	15
16	Highly Substituted Î”³â€1,2,3â€Triazolines: Solidâ€State Emitters with Electrofluorochromic Behavior. Chemistry - A European Journal, 2019, 25, 6718-6721.	1.7	10
17	Quantum Chemistry Meets Machine Learning. Chimia, 2019, 73, 983.	0.3	8
18	Transferable Machine-Learning Model of the Electron Density. ACS Central Science, 2019, 5, 57-64.	5.3	178

#	Article	IF	Citations
19	The role of bridging ligands in dinitrogen reduction and functionalization by uranium multimetallic complexes. Nature Chemistry, 2019, 11, 154-160.	6.6	100
20	How do London Dispersion Interactions Impact the Photochemical Processes of Molecular Switches?. Journal of Physical Chemistry Letters, 2018, 9, 464-470.	2.1	22
21	Exploring the Limitation of Molecular Water Oxidation Catalysts. Journal of Physical Chemistry C, 2018, 122, 12404-12412.	1.5	37
22	Synthesis and characterization of semiaromatic polyamides comprising benzofurobenzofuran repeating units. Polymer Chemistry, 2017, 8, 2197-2209.	1.9	14
23	Quantum Chemical Study of the Water Exchange Mechanism of the Americyl(VI) Aqua Ion. Inorganic Chemistry, 2016, 55, 11147-11152.	1.9	5
24	Rationalizing fluorescence quenching in meso-BODIPY dyes. Physical Chemistry Chemical Physics, 2016, 18, 32668-32672.	1.3	48
25	Qualitatively Incorrect Features in the TDDFT Spectrum of Thiophene-Based Compounds. Journal of Physical Chemistry Letters, 2015, 6, 13-21.	2.1	62