Barbara Fresch

List of Publications by Year in descending order

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567281 752698 39 458 15 20 citations h-index g-index papers 41 41 41 656 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	Ligand and Solvation Effects on the Structural and Electronic Properties of Small Gold Clusters. Journal of Physical Chemistry C, 2014, 118, 4362-4376.	3.1	34
2	Charge Redistribution Effects on the UV–Vis Spectra of Small Ligated Gold Clusters: a Computational Study. Journal of Physical Chemistry C, 2015, 119, 10969-10980.	3.1	33
3	A Cu(<scp>ii</scp>) complex targeting the translocator protein: in vitro and in vivo antitumor potential and mechanistic insights. Chemical Communications, 2017, 53, 134-137.	4.1	30
4	Molecular decision trees realized by ultrafast electronic spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 17183-17188.	7.1	26
5	Parallel and Multivalued Logic by the Two-Dimensional Photon-Echo Response of a Rhodamine–DNA Complex. Journal of Physical Chemistry Letters, 2015, 6, 1714-1718.	4.6	26
6	Reactivity of Auranofin with Selenols and Thiols – Implications for the Anticancer Activity of Gold(I) Compounds. European Journal of Inorganic Chemistry, 2013, 2013, 2718-2727.	2.0	25
7	Coherent electronic and nuclear dynamics in a rhodamine heterodimer–DNA supramolecular complex. Physical Chemistry Chemical Physics, 2017, 19, 23043-23051.	2.8	24
8	Fast Energy Transfer in CdSe Quantum Dot Layered Structures: Controlling Coupling with Covalent-Bond Organic Linkers. Journal of Physical Chemistry C, 2018, 122, 5753-5758.	3.1	22
9	Typicality in Ensembles of Quantum States: Monte Carlo Sampling versus Analytical Approximations. Journal of Physical Chemistry A, 2009, 113, 14502-14513.	2.5	20
10	Tuning the Properties of Pd Nanoclusters by Ligand Coatings: Electronic Structure Computations on Phosphine, Thiol, and Mixed Phosphine–Thiol Ligand Shells. Journal of Physical Chemistry C, 2014, 118, 9790-9800.	3.1	20
11	Magnetostructural effects in ligand stabilized Pd13 clusters: a density functional theory study. Nanoscale, 2012, 4, 4138.	5.6	17
12	Atomistic account of structural and dynamical changes induced by small binders in the double helix of a short DNA. Physical Chemistry Chemical Physics, 2014, 16, 14070-14082.	2.8	17
13	Interplay of structural and electronic stabilizing factors in neutral and cationic phosphine protected Au13 clusters. European Physical Journal D, 2012, 66, 1.	1.3	16
14	Emergence of equilibrium thermodynamic properties in quantum pure states. II. Analysis of a spin model system. Journal of Chemical Physics, 2010, 133, 034510.	3.0	15
15	Emergence of equilibrium thermodynamic properties in quantum pure states. I. Theory. Journal of Chemical Physics, 2010, 133, 034509.	3.0	15
16	Coherent Exciton Dynamics in Ensembles of Size-Dispersed CdSe Quantum Dot Dimers Probed via Ultrafast Spectroscopy: A Quantum Computational Study. Applied Sciences (Switzerland), 2020, 10, 1328.	2.5	12
17	Force measurements reveal how small binders perturb the dissociation mechanisms of DNA duplex sequences. Nanoscale, 2016, 8, 11718-11726.	5.6	11
18	Typical response of quantum pure states. European Physical Journal B, 2013, 86, 1.	1.5	10

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19	Information processing in parallel through directionally resolved molecular polarization components in coherent multidimensional spectroscopy. Journal of Chemical Physics, 2015, 143, 064106.	3.0	10
20	Effect of Different Conformational Distributions on the Ultrafast Coherence Dynamics in Porphyrin-Based Polymers. Journal of Physical Chemistry C, 2019, 123, 10212-10224.	3.1	10
21	Beyond quantum microcanonical statistics. Journal of Chemical Physics, 2011, 134, 054510.	3.0	9
22	A Probabilistic Finite State Logic Machine Realized Experimentally on a Single Dopant Atom. Nano Letters, 2017, 17, 1846-1852.	9.1	9
23	Collective Fluctuations in Ordered Fluids Investigated by Two-Dimensional Electronâ´'Electron Double Resonance Spectroscopy. Journal of Physical Chemistry B, 2006, 110, 24238-24254.	2.6	6
24	Spectral shift, electronic coupling and exciton delocalization in nanocrystal dimers: insights from all-atom electronic structure computations. Nanoscale, 2020, 12, 18124-18136.	5.6	6
25	Quantum computing for classical problems: variational quantum eigensolver for activated processes. New Journal of Physics, 2021, 23, 123045.	2.9	5
26	Pilot-Wave Quantum Theory with a Single Bohm's Trajectory. Foundations of Physics, 2016, 46, 575-605.	1.3	4
27	Multivalued Logic at the Nanoscale. Natural Computing Series, 2018, , 295-318.	2.2	4
28	Stability of antibacterial Te(IV) compounds: A combined experimental and computational study. Journal of Inorganic Biochemistry, 2019, 198, 110719.	3.5	4
29	Strategies to simulate dephasing-assisted quantum transport on digital quantum computers. New Journal of Physics, 2022, 24, 023039.	2.9	4
30	Implementation of Multivariable Logic Functions in Parallel by Electrically Addressing a Molecule of Three Dopants in Silicon. ChemPhysChem, 2017, 18, 1790-1797.	2.1	3
31	Querying a quasi-classical Oracle: One-bit function identification problem implemented in a single atom transistor. Europhysics Letters, 2012, 99, 28004.	2.0	2
32	Implementation of Probabilistic Algorithms by Multiâ€chromophoric Molecular Networks with Application to Multiple Travelling Pathways. ChemPhysChem, 2017, 18, 1782-1789.	2.1	2
33	Chirality of a rhodamine heterodimer linked to a DNA scaffold: an experimental and computational study. Physical Chemistry Chemical Physics, 2020, 22, 7516-7523.	2.8	2
34	Quantum Statistical Ensemble Resilient to Thermalization. Journal of Physical Chemistry A, 2016, 120, 5071-5082.	2.5	1
35	Thermal Pure States for Finite and Isolated Quantum Systems. Journal of Physical Chemistry A, 2017, 121, 7261-7272.	2.5	1
36	Signatures of Anderson localization and delocalized random quantum states. Chemical Physics, 2018, 514, 141-149.	1.9	1

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37	The tunneling splitting and the Kramers theory of activated processes. Chemical Physics, 2022, 561, 111608.	1.9	1
38	An n-Bit Adder Realized via Coherent Optical Parallel Computing. , 2019, , .		0
39	Electronic coherences in rhodamine dimers: vibronic coupling and distance dependence., 2016,,.		O