Ruth Pachter

List of Publications by Year
in descending order

47 papers	1,444 citations	394286 19 h-index	330025 37 g-index
47 all docs	47 docs citations	47 times ranked	1888 citing authors

#	Article	IF	Citations
1	The joint automated repository for various integrated simulations (JARVIS) for data-driven materials design. Npj Computational Materials, 2020, 6, .	3.5	181
2	Halogen Etch of Ti₃AlC₂ MAX Phase for MXene Fabrication. ACS Nano, 2021, 15, 2771-2777.	7.3	154
3	Understanding Structural and Optical Properties of Nanoscale CdSe Magic-Size Quantum Dots: Insight from Computational Prediction. Journal of Physical Chemistry C, 2010, 114, 16197-16209.	1.5	115
4	TDDFT Study of One- and Two-Photon Absorption Properties:Â Donorâˆ'Ï€âˆ'Acceptor Chromophores. Journal of Physical Chemistry B, 2005, 109, 1803-1814.	1.2	101
5	Accelerated Discovery of Efficient Solar Cell Materials Using Quantum and Machine-Learning Methods. Chemistry of Materials, 2019, 31, 5900-5908.	3.2	87
6	Design Parameters for Tuning the Type 1 Cu Multicopper Oxidase Redox Potential: Insight from a Combination of First Principles and Empirical Molecular Dynamics Simulations. Journal of the American Chemical Society, 2011, 133, 4802-4809.	6.6	81
7	Calculation of two-photon absorption spectra of donor-Ï€-acceptor compounds in solution using quadratic response time-dependent density functional theory. Journal of Chemical Physics, 2006, 125, 094103.	1.2	63
8	Electron-Withdrawing Effect of Native Terminal Groups on the Lattice Structure of Ti₃C₂T_x MXenes Studied by Resonance Raman Scattering: Implications for Embedding MXenes in Electronic Composites. ACS Applied Nano Materials, 2019, 2, 6087-6091.	2.4	55
9	Computational Prediction of Structures and Optical Excitations for Nanoscale Ultrasmall ZnS and CdSe Clusters. Journal of Chemical Theory and Computation, 2013, 9, 3581-3596.	2.3	51
10	Calculation of One- and Two-Photon Absorption Spectra of Thiolated Gold Nanoclusters using Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2010, 6, 2809-2821.	2.3	47
11	Extrinsic Dopant Effects on Oxygen Vacancy Formation Energies in ZrO₂ with Implication for Memristive Device Performance. ACS Applied Electronic Materials, 2019, 1, 467-477.	2.0	38
12	Computational search for magnetic and non-magnetic 2D topological materials using unified spinâ€“orbit spillage screening. Npj Computational Materials, 2020, 6, .	3.5	32
13	Linear and Nonlinear Optical Response in Silver Nanoclusters: Insight from a Computational Investigation. Journal of Physical Chemistry A, 2016, 120, 507-518.	1.1	31
14	Mechanistic Analysis of Oxygen Vacancy-Driven Conductive Filament Formation in Resistive Random Access Memory Metal/NiO/Metal Structures. ACS Applied Materials & Interfaces, 2018, 10, 9802-9816.	4.0	29
15	One- and Two-Photon Spectra of Platinum Acetylide Chromophores: A TDDFT Study. Journal of Physical Chemistry A, 2009, 113, 13943-13952.	1.1	28
16	Toward Architected Nanocomposites: MXenes and Beyond. ACS Nano, 2021, 15, 21-28.	7.3	28
17	Calculation of One-Photon and Two-Photon Absorption Spectra of Porphyrins Using Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2008, 4, 1094-1106.	2.3	27
18	Interlayerâ€Sensitized Linear and Nonlinear Photoluminescence of Quasiâ€2D Hybrid Perovskites Using Aggregationâ€Induced Enhanced Emission Active Organic Cation Layers. Advanced Functional Materials, 2020, 30, 1909375.	7.8	21

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19	Interstitial Nature of Mn²⁺ Doping in 2D Perovskites. ACS Nano, 2021, 15, 20550-20561.	7.3	19
20	Theoretical analysis of structures and electronic spectra in molecular cadmium chalcogenide clusters. Journal of Chemical Physics, 2015, 142, 234305.	1.2	18
21	Surface Functionalization of Ti₃C₂T_x MXene Nanosheets with Catechols: Implication for Colloidal Processing. Langmuir, 2021, 37, 5447-5456.	1.6	17
22	Tunability in the optical response of defective monolayer WSe₂ by computational analysis. Nanoscale, 2018, 10, 13751-13760.	2.8	16
23	Second-Order Nonlinear Optical Properties of Monolayer Transition-Metal Dichalcogenides by Computational Analysis. Journal of Physical Chemistry C, 2021, 125, 11075-11084.	1.5	16
24	Defect engineering of graphene using electron-beam chemistry with radiolyzed water. Carbon, 2020, 166, 446-455.	5.4	15
25	Effects of exciton-plasmon strong coupling on third harmonic generation by two-dimensional WS2 at periodic plasmonic interfaces. Journal of Chemical Physics, 2018, 148, .	1.2	14
26	Photoactivation of Cryptochromes from Drosophila melanogaster and Sylvia borin: Insight into the Chemical Compass Mechanism by Computational Investigation. Journal of Physical Chemistry B, 2015, 119, 3883-3892.	1.2	13
27	Electron transfer and spin dynamics of the radical-pair in the cryptochrome from Chlamydomonas reinhardtii by computational analysis. Journal of Chemical Physics, 2020, 152, 065101.	1.2	13
28	Dependence of the Electronic and Optical Properties of Methylammonium Lead Triiodide on Ferroelectric Polarization Directions and Domains: A First Principles Computational Study. Journal of Physical Chemistry C, 2017, 121, 15375-15383.	1.5	11
29	Systematic Study of Structure, Stability, and Electronic Absorption of Tetrahedral CdSe Clusters with Carboxylate and Amine Ligands. Journal of Physical Chemistry A, 2018, 122, 6704-6712.	1.1	10
30	Describing a Strongly Correlated Model System with Density Functional Theory. Journal of Physical Chemistry Letters, 2017, 8, 3142-3146.	2.1	9
31	Theoretical Prediction of Optical Absorption and Emission in Thiolated Gold Clusters. Journal of Physical Chemistry A, 2019, 123, 6472-6481.	1.1	9
32	Harmonic Generation by Metal Nanostructures Optically Coupled to Two-Dimensional Transition-Metal Dichalcogenide. Journal of Physical Chemistry C, 2019, 123, 6898-6904.	1.5	9
33	Systematic Study of the Properties of CdS Clusters with Carboxylate Ligands Using a Deep Neural Network Potential Developed with Data from Density Functional Theory Calculations. Journal of Physical Chemistry A, 2020, 124, 10472-10481.	1.1	9
34	Coupling Drosophila melanogaster Cryptochrome Light Activation and Oxidation of the Kv$\hat{I}^2$ Subunit Hyperkinetic NADPH Cofactor. Journal of Physical Chemistry B, 2018, 122, 6503-6510.	1.2	8
35	Two-dimensional MoS₂2H, 1T, and 1T^{â€²}crystalline phases with incorporated adatoms: theoretical investigation of electronic and optical properties. Applied Optics, 2021, 60, G232.	0.9	8
36	Electrical and chemical properties of vacancy-ordered lead free layered double perovskite nanoparticles. Nanoscale, 2022, 14, 3487-3495.	2.8	8

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37	Predicting Van der Waals Heterostructures by a Combined Machine Learning and Density Functional Theory Approach. ACS Applied Materials & Interfaces, 2022, 14, 25907-25919.	4.0	8
38	A Theoretical Investigation of the Structure and Optical Properties of a Silver Cluster in Solid Form and in Solution. Journal of Physical Chemistry A, 2017, 121, 326-333.	1.1	7
39	Computational design of two-photon active organic molecules for infrared responsive materials. Journal of Materials Chemistry C, 2020, 8, 9867-9873.	2.7	7
40	Hybrid Organic Lead Iodides: Role of Organic Cation Structure in Obtaining 1D Chains of Face-Sharing Octahedra vs 2D Perovskites. Chemistry of Materials, 2022, 34, 935-946.	3.2	7
41	Calculations of One- and Two-Photon Absorption Spectra for Molecular Metal Chalcogenide Clusters with Electron-Acceptor Ligands. Journal of Physical Chemistry A, 2017, 121, 1748-1759.	1.1	5
42	Theoretical Analysis of Optical Absorption and Emission in Mixed Noble Metal Nanoclusters. Journal of Physical Chemistry A, 2018, 122, 4058-4066.	1.1	5
43	Elucidating the Role of the Organic Cation in Tuning the Optical Response of Two-Dimensional Organicâ€“Inorganic Halide Perovskites by Computational Investigation. Journal of Physical Chemistry C, 2020, 124, 3224-3232.	1.5	4
44	Theoretical analysis of structures and electronic spectra of molecular colloidal cadmium sulfide clusters and nanoplatelets. Journal of Chemical Physics, 2021, 155, 094302.	1.2	4
45	Computational analysis of the optical response of ZnSe with d-orbital defects. Journal of Physics Condensed Matter, 2022, 34, 205402.	0.7	3
46	Patterned graphene: Analysis of the electronic structure and electron transport by first principles computational modeling. Applied Surface Science, 2022, 589, 152953.	3.1	2
47	Calculated linear and nonlinear optical absorption spectra of phosphine-ligated gold clusters. Physical Chemistry Chemical Physics, 2022, 24, 11234-11248.	1.3	1