

Robert A Distasio Jr

List of Publications by Year in descending order

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61
papers

13,498
citations

87843

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docs citations

65
times ranked

13463
citing authors

#	ARTICLE	IF	CITATIONS
1	Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies. <i>Chemical Reviews</i> , 2022, 122, 6117-6321.	23.0	195
2	Expeditious synthesis of aromatic-free piperidinium-functionalized polyethylene as alkaline anion exchange membranes. <i>Chemical Science</i> , 2021, 12, 3898-3910.	3.7	47
3	QM7-X, a comprehensive dataset of quantum-mechanical properties spanning the chemical space of small organic molecules. <i>Scientific Data</i> , 2021, 8, 43.	2.4	46
4	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
5	Electron confinement meet electron delocalization: non-additivity and finite-size effects in the polarizabilities and dispersion coefficients of the fullerenes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 5773-5779.	1.3	4
6	Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory-Based <i>Ab Initio</i> Molecular Dynamics II: Extensions to the Isobaric-Isoenthalpic and Isobaric-Isothermal Ensembles. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7789-7813.	2.3	7
7	NENCI-2021. I. A large benchmark database of non-equilibrium non-covalent interactions emphasizing close intermolecular contacts. <i>Journal of Chemical Physics</i> , 2021, 155, 184303.	1.2	15
8	Predicting molecular dipole moments by combining atomic partial charges and atomic dipoles. <i>Journal of Chemical Physics</i> , 2020, 153, 024113.	1.2	65
9	Area-selective atomic layer deposition enabled by competitive adsorption. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2020, 38, 062411.	0.9	8
10	Oxyaapa: A Picolinate-Based Ligand with Five Oxygen Donors that Strongly Chelates Lanthanides. <i>Inorganic Chemistry</i> , 2020, 59, 5116-5132.	1.9	14
11	Attracting Opposites: Promiscuous Ion Binding in the Nucleobases. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4128-4140.	1.1	3
12	Tuning the Mechanical Properties of Metallopolymers via Ligand Interactions: A Combined Experimental and Theoretical Study. <i>Macromolecules</i> , 2020, 53, 2021-2030.	2.2	18
13	Dual electrocatalysis enables enantioselective hydrocyanation of conjugated alkenes. <i>Nature Chemistry</i> , 2020, 12, 747-754.	6.6	176
14	Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory Based <i>Ab Initio</i> Molecular Dynamics. I. Theory, Algorithm, and Performance. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3757-3785.	2.3	29
15	Competitive Adsorption as a Route to Area-Selective Deposition. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 9989-9999.	4.0	14
16	Isotope effects in liquid water via deep potential molecular dynamics. <i>Molecular Physics</i> , 2019, 117, 3269-3281.	0.8	52
17	Quantum mechanical static dipole polarizabilities in the QM7b and AlphaML showcase databases. <i>Scientific Data</i> , 2019, 6, 152.	2.4	20
18	Accurate molecular polarizabilities with coupled cluster theory and machine learning. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 3401-3406.	3.3	126

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19	Influence of Pore Size on the van der Waals Interaction in Two-Dimensional Molecules and Materials. <i>Physical Review Letters</i> , 2019, 122, 026001.	2.9	11
20	Reliable and practical computational description of molecular crystal polymorphs. <i>Science Advances</i> , 2019, 5, eaau3338.	4.7	127
21	Rational design of stealthy hyperuniform two-phase media with tunable order. <i>Physical Review E</i> , 2018, 97, 023311.	0.8	17
22	Coherent, atomically thin transition-metal dichalcogenide superlattices with engineered strain. <i>Science</i> , 2018, 359, 1131-1136.	6.0	247
23	Exploiting Molecular Weight Distribution Shape to Tune Domain Spacing in Block Copolymer Thin Films. <i>Journal of the American Chemical Society</i> , 2018, 140, 4639-4648.	6.6	99
24	Non-covalent interactions across organic and biological subsets of chemical space: Physics-based potentials parametrized from machine learning. <i>Journal of Chemical Physics</i> , 2018, 148, 241706.	1.2	136
25	Hydroxide diffuses slower than hydronium in water because its solvated structure inhibits correlated proton transfer. <i>Nature Chemistry</i> , 2018, 10, 413-419.	6.6	175
26	Perturbed path integrals in imaginary time: Efficiently modeling nuclear quantum effects in molecules and materials. <i>Journal of Chemical Physics</i> , 2018, 148, 102325.	1.2	10
27	On the geometric dependence of the molecular dipole polarizability in water: A benchmark study of higher-order electron correlation, basis set incompleteness error, core electron effects, and zero-point vibrational contributions. <i>Journal of Chemical Physics</i> , 2018, 149, 204303.	1.2	11
28	Unraveling substituent effects on the glass transition temperatures of biorenewable polyesters. <i>Nature Communications</i> , 2018, 9, 2880.	5.8	58
29	Thermal expansion in dispersion-bound molecular crystals. <i>Physical Review Materials</i> , 2018, 2, .	0.9	18
30	First-Principles Models for van der Waals Interactions in Molecules and Materials: Concepts, Theory, and Applications. <i>Chemical Reviews</i> , 2017, 117, 4714-4758.	23.0	408
31	eQE: An open-source density functional embedding theory code for the condensed phase. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25401.	1.0	40
32	Report on the sixth blind test of organic crystal structure prediction methods. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 439-459.	0.5	445
33	Inverse design of disordered stealthy hyperuniform spin chains. <i>Physical Review B</i> , 2016, 93, .	1.1	14
34	Wavelike charge density fluctuations and van der Waals interactions at the nanoscale. <i>Science</i> , 2016, 351, 1171-1176.	6.0	217
35	Analytical nuclear gradients for the range-separated many-body dispersion model of noncovalent interactions. <i>Chemical Science</i> , 2016, 7, 1712-1728.	3.7	33
36	A systematic study of chloride ion solvation in water using van der Waals inclusive hybrid density functional theory. <i>Molecular Physics</i> , 2015, 113, 2842-2854.	0.8	47

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37	Local structure analysis in <i>ab initio</i> liquid water. <i>Molecular Physics</i> , 2015, 113, 2829-2841.	0.8	96
38	Numerical Study on the Partitioning of the Molecular Polarizability into Fluctuating Charge and Induced Atomic Dipole Contributions. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5865-5882.	1.1	44
39	Electronic Properties of Molecules and Surfaces with a Self-Consistent Interatomic van der Waals Density Functional. <i>Physical Review Letters</i> , 2015, 114, 176802.	2.9	79
40	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	0.8	2,561
41	Shared memory multiprocessing implementation of resolution-of-the-identity second-order Møller-Plesset perturbation theory with attenuated and unattenuated results for intermolecular interactions between large molecules. <i>Molecular Physics</i> , 2014, 112, 836-843.	0.8	10
42	The individual and collective effects of exact exchange and dispersion interactions on the <i>ab initio</i> structure of liquid water. <i>Journal of Chemical Physics</i> , 2014, 141, 084502.	1.2	276
43	Long-range correlation energy calculated from coupled atomic response functions. <i>Journal of Chemical Physics</i> , 2014, 140, 18A508.	1.2	480
44	Hard Numbers for Large Molecules: Toward Exact Energetics for Supramolecular Systems. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 849-855.	2.1	159
45	Many-body van der Waals interactions in molecules and condensed matter. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 213202.	0.7	190
46	Interatomic methods for the dispersion energy derived from the adiabatic connection fluctuation-dissipation theorem. <i>Journal of Chemical Physics</i> , 2013, 138, 074106.	1.2	129
47	Many-Body Dispersion Interactions in Molecular Crystal Polymorphism. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 6629-6632.	7.2	149
48	Designer spin systems via inverse statistical mechanics. II. Ground-state enumeration and classification. <i>Physical Review B</i> , 2013, 88, .	1.1	7
49	Designer spin systems via inverse statistical mechanics. <i>Physical Review B</i> , 2013, 88, .	1.1	14
50	Accurate and Efficient Method for Many-Body van der Waals Interactions. <i>Physical Review Letters</i> , 2012, 108, 236402.	2.9	1,120
51	Collective many-body van der Waals interactions in molecular systems. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 14791-14795.	3.3	178
52	Current Status of the AMOEBA Polarizable Force Field. <i>Journal of Physical Chemistry B</i> , 2010, 114, 2549-2564.	1.2	1,093
53	The 1,4-phenylenediisocyanide dimer: gas-phase properties and insights into organic self-assembled monolayers. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 82-96.	1.3	4
54	Dispersion-corrected Møller-Plesset second-order perturbation theory. <i>Journal of Chemical Physics</i> , 2009, 131, 094106.	1.2	223

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55	Non-Covalent Interactions with Dual-Basis Methods: Pairings for Augmented Basis Sets. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1560-1572.	2.3	39
56	The analytical gradient of dual-basis resolution-of-the-identity second-order Møller-Plesset perturbation theory. <i>Molecular Physics</i> , 2007, 105, 2731-2742.	0.8	31
57	Optimized spin-component scaled second-order Møller-Plesset perturbation theory for intermolecular interaction energies. <i>Molecular Physics</i> , 2007, 105, 1073-1083.	0.8	225
58	An improved algorithm for analytical gradient evaluation in resolution-of-the-identity second-order Møller-Plesset perturbation theory: Application to alanine tetrapeptide conformational analysis. <i>Journal of Computational Chemistry</i> , 2007, 28, 839-856.	1.5	134
59	Advances in methods and algorithms in a modern quantum chemistry program package. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 3172-3191.	1.3	2,597
60	Dual-basis second-order Møller-Plesset perturbation theory: A reduced-cost reference for correlation calculations. <i>Journal of Chemical Physics</i> , 2006, 125, 074108.	1.2	90
61	A Resolution-Of-The-Identity Implementation of the Local Triatomics-In-Molecules Model for Second-Order Møller-Plesset Perturbation Theory with Application to Alanine Tetrapeptide Conformational Energies. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 862-876.	2.3	90