Robert A Distasio Jr

List of Publications by Year
in descending order

61 papers	13,498 citations	87888 38 h-index	114465 63 g-index
65 all docs	65 docs citations	65 times ranked	13463 citing authors

#	Article	IF	Citations
1	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	2.8	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
3	Accurate and Efficient Method for Many-Body van der Waals Interactions. Physical Review Letters, 2012, 108, 236402.	7.8	1,120
4	Current Status of the AMOEBA Polarizable Force Field. Journal of Physical Chemistry B, 2010, 114, 2549-2564.	2.6	1,093
5	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
6	Long-range correlation energy calculated from coupled atomic response functions. Journal of Chemical Physics, 2014, 140, 18A508.	3.0	480
7	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	1.1	445
8	First-Principles Models for van der Waals Interactions in Molecules and Materials: Concepts, Theory, and Applications. Chemical Reviews, 2017, 117, 4714-4758.	47.7	408
9	The individual and collective effects of exact exchange and dispersion interactions on the ab initio structure of liquid water. Journal of Chemical Physics, 2014, 141, 084502.	3.0	276
10	Coherent, atomically thin transition-metal dichalcogenide superlattices with engineered strain. Science, 2018, 359, 1131-1136.	12.6	247
11	Optimized spin-component scaled second-order MÃ¸ller-Plesset perturbation theory for intermolecular interaction energies. Molecular Physics, 2007, 105, 1073-1083.	1.7	225
12	Dispersion-corrected MÃ¸llerâ€“Plesset second-order perturbation theory. Journal of Chemical Physics, 2009, 131, 094106.	3.0	223
13	Wavelike charge density fluctuations and van der Waals interactions at the nanoscale. Science, 2016, 351, 1171-1176.	12.6	217
14	Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies. Chemical Reviews, 2022, 122, 6117-6321.	47.7	195
15	Many-body van der Waals interactions in molecules and condensed matter. Journal of Physics Condensed Matter, 2014, 26, 213202.	1.8	190
16	Collective many-body van der Waals interactions in molecular systems. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 14791-14795.	7.1	178
17	Dual electrocatalysis enables enantioselective hydrocyanation of conjugated alkenes. Nature Chemistry, 2020, 12, 747-754.	13.6	176
18	Hydroxide diffuses slower than hydronium in water because its solvated structure inhibits correlated proton transfer. Nature Chemistry, 2018, 10, 413-419.	13.6	175

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19	Hard Numbers for Large Molecules: Toward Exact Energetics for Supramolecular Systems. Journal of Physical Chemistry Letters, 2014, 5, 849-855.	4.6	159
20	Manyâ€Body Dispersion Interactions in Molecular Crystal Polymorphism. Angewandte Chemie - International Edition, 2013, 52, 6629-6632.	13.8	149
21	Non-covalent interactions across organic and biological subsets of chemical space: Physics-based potentials parametrized from machine learning. Journal of Chemical Physics, 2018, 148, 241706.	3.0	136
22	An improved algorithm for analytical gradient evaluation in resolution-of-the-identity second-order MÃ¸ller-Plesset perturbation theory: Application to alanine tetrapeptide conformational analysis. Journal of Computational Chemistry, 2007, 28, 839-856.	3.3	134
23	Interatomic methods for the dispersion energy derived from the adiabatic connection fluctuation-dissipation theorem. Journal of Chemical Physics, 2013, 138, 074106.	3.0	129
24	Reliable and practical computational description of molecular crystal polymorphs. Science Advances, 2019, 5, eaau3338.	10.3	127
25	Accurate molecular polarizabilities with coupled cluster theory and machine learning. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 3401-3406.	7.1	126
26	Exploiting Molecular Weight Distribution Shape to Tune Domain Spacing in Block Copolymer Thin Films. Journal of the American Chemical Society, 2018, 140, 4639-4648.	13.7	99
27	Local structure analysis in ab initio liquid water. Molecular Physics, 2015, 113, 2829-2841.	1.7	96
28	A Resolution-Of-The-Identity Implementation of the Local Triatomics-In-Molecules Model for Second-Order MÃ¸llerâ€"Plesset Perturbation Theory with Application to Alanine Tetrapeptide Conformational Energies. Journal of Chemical Theory and Computation, 2005, 1, 862-876.	5.3	90
29	Dual-basis second-order MÃ¸ller-Plesset perturbation theory: A reduced-cost reference for correlation calculations. Journal of Chemical Physics, 2006, 125, 074108.	3.0	90
30	Electronic Properties of Molecules and Surfaces with a Self-Consistent Interatomic van der Waals Density Functional. Physical Review Letters, 2015, 114, 176802.	7.8	79
31	Predicting molecular dipole moments by combining atomic partial charges and atomic dipoles. Journal of Chemical Physics, 2020, 153, 024113.	3.0	65
32	Unraveling substituent effects on the glass transition temperatures of biorenewable polyesters. Nature Communications, 2018, 9, 2880.	12.8	58
33	Isotope effects in liquid water via deep potential molecular dynamics. Molecular Physics, 2019, 117, 3269-3281.	1.7	52
34	A systematic study of chloride ion solvation in water using van der Waals inclusive hybrid density functional theory. Molecular Physics, 2015, 113, 2842-2854.	1.7	47
35	Expeditious synthesis of aromatic-free piperidinium-functionalized polyethylene as alkaline anion exchange membranes. Chemical Science, 2021, 12, 3898-3910.	7.4	47
36	QM7-X, a comprehensive dataset of quantum-mechanical properties spanning the chemical space of small organic molecules. Scientific Data, 2021, 8, 43.	5.3	46

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37	Numerical Study on the Partitioning of the Molecular Polarizability into Fluctuating Charge and Induced Atomic Dipole Contributions. Journal of Physical Chemistry A, 2015, 119, 5865-5882.	2.5	44
38	eQE: An openâ€source density functional embedding theory code for the condensed phase. International Journal of Quantum Chemistry, 2017, 117, e25401.	2.0	40
39	Non-Covalent Interactions with Dual-Basis Methods: Pairings for Augmented Basis Sets. Journal of Chemical Theory and Computation, 2009, 5, 1560-1572.	5.3	39
40	Analytical nuclear gradients for the range-separated many-body dispersion model of noncovalent interactions. Chemical Science, 2016, 7, 1712-1728.	7.4	33
41	The analytical gradient of dual-basis resolution-of-the-identity second-order MÃ¸llerâ€“Plesset perturbation theory. Molecular Physics, 2007, 105, 2731-2742.	1.7	31
42	Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics. 1. Theory, Algorithm, and Performance. Journal of Chemical Theory and Computation, 2020, 16, 3757-3785.	5.3	29
43	Quantum mechanical static dipole polarizabilities in the QM7b and AlphaML showcase databases. Scientific Data, 2019, 6, 152.	5.3	20
44	Tuning the Mechanical Properties of Metallopolymers via Ligand Interactions: A Combined Experimental and Theoretical Study. Macromolecules, 2020, 53, 2021-2030.	4.8	18
45	Thermal expansion in dispersion-bound molecular crystals. Physical Review Materials, 2018, 2, .	2.4	18
46	Rational design of stealthy hyperuniform two-phase media with tunable order. Physical Review E, 2018, 97, 023311.	2.1	17
47	NENCI-2021. I. A large benchmark database of non-equilibrium non-covalent interactions emphasizing close intermolecular contacts. Journal of Chemical Physics, 2021, 155, 184303.	3.0	15
48	Designer spin systems via inverse statistical mechanics. Physical Review B, 2013, 88, .	3.2	14
49	Inverse design of disordered stealthy hyperuniform spin chains. Physical Review B, 2016, 93, .	3.2	14
50	Oxyaapa: A Picolinate-Based Ligand with Five Oxygen Donors that Strongly Chelates Lanthanides. Inorganic Chemistry, 2020, 59, 5116-5132.	4.0	14
51	Competitive Adsorption as a Route to Area-Selective Deposition. ACS Applied Materials & Interfaces, 2020, 12, 9989-9999.	8.0	14
52	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. Journal of Chemical Physics, 2018, 149, 204303.	3.0	11
53	Influence of Pore Size on the van der Waals Interaction in Two-Dimensional Molecules and Materials. Physical Review Letters, 2019, 122, 026001.	7.8	11
54	Shared memory multiprocessing implementation of resolution-of-the-identity second-order MÃ¸llerâ€“Plesset perturbation theory with attenuated and unattenuated results for intermolecular interactions between large molecules. Molecular Physics, 2014, 112, 836-843.	1.7	10

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55	Perturbed path integrals in imaginary time: Efficiently modeling nuclear quantum effects in molecules and materials. Journal of Chemical Physics, 2018, 148, 102325.	3.0	10
56	Area-selective atomic layer deposition enabled by competitive adsorption. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2020, 38, 062411.	2.1	8
57	Designer spin systems via inverse statistical mechanics. II. Ground-state enumeration and classification. Physical Review B, 2013, 88, .	3.2	7
58	Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory-Based Ab Initio Molecular Dynamics II: Extensions to the Isobaricâ€“Isoenthalpic and Isobaricâ€“Isothermal Ensembles. Journal of Chemical Theory and Computation, 2021, 17, 7789-7813.	5.3	7
59	The 1,4-phenylenediisocyanide dimer: gas-phase properties and insights into organic self-assembled monolayers. Physical Chemistry Chemical Physics, 2010, 12, 82-96.	2.8	4
60	Electron confinement meet electron delocalization: non-additivity and finite-size effects in the polarizabilities and dispersion coefficients of the fullerenes. Physical Chemistry Chemical Physics, 2021, 23, 5773-5779.	2.8	4
61	Attracting Opposites: Promiscuous Ionâ˜Ï€ Binding in the Nucleobases. Journal of Physical Chemistry A, 2020, 124, 4128-4140.	2.5	3