Narbe Mardirossian

List of Publications by Year
in descending order

21	7,124	471061 17	642321 23
papers	citations	h-index	g-index

24	24	24	6745
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
2	Assessment of Density Functional Theory in Predicting Interaction Energies between Water and Polycyclic Aromatic Hydrocarbons: from Water on Benzene to Water on Graphene. Journal of Chemical Theory and Computation, 2019, 15, 2359-2374.	2.3	18
3	Lowering of the complexity of quantum chemistry methods by choice of representation. Journal of Chemical Physics, 2018, 148, 044106.	1.2	22
4	Survival of the most transferable at the top of Jacobâ€™s ladder: Defining and testing the Ï‰B97M(2) double hybrid density functional. Journal of Chemical Physics, 2018, 148, 241736.	1.2	136
5	Ab initio molecular dynamics simulations of liquid water using high quality meta-GGA functionals. Chemical Science, 2017, 8, 3554-3565.	3.7	95
6	Thirty years of density functional theory in computational chemistry: an overview and extensive assessment of 200 density functionals. Molecular Physics, 2017, 115, 2315-2372.	0.8	1,401
7	Use of the rVV10 Nonlocal Correlation Functional in the B97M-V Density Functional: Defining B97M-rV and Related Functionals. Journal of Physical Chemistry Letters, 2017, 8, 35-40.	2.1	78
8	Toward chemical accuracy in the description of ionâ€“water interactions through many-body representations. Alkali-water dimer potential energy surfaces. Journal of Chemical Physics, 2017, 147, 161715.	1.2	57
9	Self-consistent implementation of meta-GGA functionals for the ONETEP linear-scaling electronic structure package. Journal of Chemical Physics, 2016, 145, 204114.	1.2	18
10	Note: The performance of new density functionals for a recent blind test of non-covalent interactions. Journal of Chemical Physics, 2016, 145, 186101.	1.2	11
11	Ï‰B97M-V: A combinatorially optimized, range-separated hybrid, meta-GGA density functional with VV10 nonlocal correlation. Journal of Chemical Physics, 2016, 144, 214110.	1.2	595
12	Approaching the basis set limit for DFT calculations using an environment-adapted minimal basis with perturbation theory: Formulation, proof of concept, and a pilot implementation. Journal of Chemical Physics, 2016, 145, 044109.	1.2	16
13	How Accurate Are the Minnesota Density Functionals for Noncovalent Interactions, Isomerization Energies, Thermochemistry, and Barrier Heights Involving Molecules Composed of Main-Group Elements?. Journal of Chemical Theory and Computation, 2016, 12, 4303-4325.	2.3	355
14	Fast, accurate evaluation of exact exchange: The occ-RI-K algorithm. Journal of Chemical Physics, 2015, 143, 024113.	1.2	44
15	Mapping the genome of meta-generalized gradient approximation density functionals: The search for B97M-V. Journal of Chemical Physics, 2015, 142, 074111.	1.2	305
16	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
17	Exploring the limit of accuracy for density functionals based on the generalized gradient approximation: Local, global hybrid, and range-separated hybrid functionals with and without dispersion corrections. Journal of Chemical Physics, 2014, 140, 18A527.	1.2	34
18	Ï‰B97X-V: A 10-parameter, range-separated hybrid, generalized gradient approximation density functional with nonlocal correlation, designed by a survival-of-the-fittest strategy. Physical Chemistry Chemical Physics, 2014, 16, 9904.	1.3	616

#	Article	IF	Citations
19	Characterizing and Understanding the Remarkably Slow Basis Set Convergence of Several Minnesota Density Functionals for Intermolecular Interaction Energies. Journal of Chemical Theory and Computation, 2013, 9, 4453-4461.	2.3	83
20	The Performance of Density Functionals for Sulfateâ€“Water Clusters. Journal of Chemical Theory and Computation, 2013, 9, 1368-1380.	2.3	69
21	Benchmark results for empirical post-GGA functionals: Difficult exchange problems and independent tests. Physical Chemistry Chemical Physics, 2011, 13, 19325.	1.3	83