Alejandro J Garza

List of Publications by Year
in descending order

29 papers	1,987 citations	361413 20 h-index	477307 29 g-index
29 all docs	29 docs citations	29 times ranked	2851 citing authors

#	Article	IF	Citations
1	Assessing combinations of singlet-paired coupled cluster and density functional theory for treating electron correlation in closed and open shells. Molecular Physics, 2020, 118, 1615144.	1.7	1
2	Solvation Entropy Made Simple. Journal of Chemical Theory and Computation, 2019, 15, 3204-3214.	5.3	42
3	Explaining the Incorporation of Oxygen Derived from Solvent Water into the Oxygenated Products of CO Reduction over Cu. Journal of the American Chemical Society, 2019, 141, 4191-4193.	13.7	29
4	Challenges in Modeling Electrochemical Reaction Energetics with Polarizable Continuum Models. ACS Catalysis, 2019, 9, 920-931.	11.2	153
5	Is Subsurface Oxygen Necessary for the Electrochemical Reduction of CO₂ on Copper?. Journal of Physical Chemistry Letters, 2018, 9, 601-606.	4.6	118
6	Mechanism of CO₂ Reduction at Copper Surfaces: Pathways to C₂ Products. ACS Catalysis, 2018, 8, 1490-1499.	11.2	608
7	Reaction mechanism of the selective reduction of CO₂ to CO by a tetraaza [Co^{II}N₄H]²⁺ complex in the presence of protons. Physical Chemistry Chemical Physics, 2018, 20, 24058-24064.	2.8	15
8	Nonempirical Meta-Generalized Gradient Approximations for Modeling Chemisorption at Metal Surfaces. Journal of Chemical Theory and Computation, 2018, 14, 3083-3090.	5.3	20
9	Electronic Structure and Properties of Berkelium Iodates. Journal of the American Chemical Society, 2017, 139, 13361-13375.	13.7	25
10	Predicting Band Gaps with Hybrid Density Functionals. Journal of Physical Chemistry Letters, 2016, 7, 4165-4170.	4.6	369
11	Intensive Atomization Energy: Re-Thinking a Metric for Electronic Structure Theory Methods. Zeitschrift Fur Physikalische Chemie, 2016, 230, 737-742.	2.8	14
12	The two pillars: density and spin-density functional theories. Molecular Physics, 2016, 114, 928-931.	1.7	6
13	Combinations of coupled cluster, density functionals, and the random phase approximation for describing static and dynamic correlation, and van der Waals interactions. Molecular Physics, 2016, 114, 997-1018.	1.7	23
14	Actinide chemistry using singlet-paired coupled cluster and its combinations with density functionals. Journal of Chemical Physics, 2015, 143, 244106.	3.0	22
15	Range separated hybrids of pair coupled cluster doubles and density functionals. Physical Chemistry Chemical Physics, 2015, 17, 22412-22422.	2.8	40
16	Synergy between pair coupled cluster doubles and pair density functional theory. Journal of Chemical Physics, 2015, 142, 044109.	3.0	36
17	On the equivalence of LIST and DIIS methods for convergence acceleration. Journal of Chemical Physics, 2015, 142, 164104.	3.0	7
18	Can Gap Tuning Schemes of Long-Range Corrected Hybrid Functionals Improve the Description of Hyperpolarizabilities?. Journal of Physical Chemistry B, 2015, 119, 1202-1212.	2.6	54

#	Article	IF	Citations
19	Can Short- and Middle-Range Hybrids Describe the Hyperpolarizabilities of Long-Range Charge-Transfer Compounds?. Journal of Physical Chemistry A, 2014, 118, 11787-11796.	2.5	52
20	The isotropic molecular polarizabilities of single methyl-branched alkanes in the terahertz range. Chemical Physics Letters, 2014, 592, 292-296.	2.6	13
21	A computational study of the nonlinear optical properties of carbazole derivatives: theory refines experiment. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	41
22	Electronic correlation without double counting via a combination of spin projected Hartree-Fock and density functional theories. Journal of Chemical Physics, 2014, 140, 244102.	3.0	26
23	Prediction of the linear and nonlinear optical properties of tetrahydronaphthalone derivatives via long-range corrected hybrid functionals. Molecular Physics, 2014, 112, 3165-3172.	1.7	21
24	Nonlinear optical properties of DPO and DMPO: a theoretical and computational study. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	24
25	Photochromic and nonlinear optical properties of fulgides: A density functional theory study. Computational and Theoretical Chemistry, 2013, 1022, 82-85.	2.5	29
26	Assessment of long-range corrected functionals for the prediction of non-linear optical properties of organic materials. Chemical Physics Letters, 2013, 575, 122-125.	2.6	62
27	Capturing static and dynamic correlations by a combination of projected Hartree-Fock and density functional theories. Journal of Chemical Physics, 2013, 138, 134102.	3.0	31
28	Conformational Preferences of trans-1,2- and cis-1,3-Cyclohexanedicarboxylic Acids in Water and Dimethyl Sulfoxide as a Function of the Ionization State As Determined from NMR Spectroscopy and Density Functional Theory Quantum Mechanical Calculations. Journal of the American Chemical Society, 2012, 134, 14772-14780.	13.7	15
29	Comparison of self-consistent field convergence acceleration techniques. Journal of Chemical Physics, 2012, 137, 054110.	3.0	91