Mark A Vincent

List of Publications by Year
in descending order

31	1,038	331670 21	434195 31
papers	citations	h-index	g-index

32	32	32	1355
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Revitalizing the concept of bond order through delocalization measures in real space. Chemical Science, 2018, 9, 5517-5529.	7.4	114
2	Mechanism of Acid Dissociation in Water Clusters:â€‰ Electronic Structure Studies of (H2O)nHX (n = 4, 7;) Tj ETQq0 0 0 rgBT /Overloc	2.5	94
3	Cooperative effects in the structuring of fluoride water clusters: Ab initio hybrid quantum mechanical/molecular mechanical model incorporating polarizable fluctuating charge solvent. Journal of Chemical Physics, 1998, 109, 3077-3085.	3.0	89
4	Density Functional and Semiempirical Molecular Orbital Methods Including Dispersion Corrections for the Accurate Description of Noncovalent Interactions Involving Sulfur-Containing Molecules. Journal of Chemical Theory and Computation, 2007, 3, 1656-1664.	5.3	73
5	Monte Carlo simulation of Fâ^'(H2O)4 using an ab initio potential. Journal of Chemical Physics, 1999, 110, 4338-4346.	3.0	54
6	Olefin Metathesis by Grubbsâ€“Hoveyda Complexes: Computational and Experimental Studies of the Mechanism and Substrate-Dependent Kinetics. ACS Catalysis, 2013, 3, 1929-1939.	11.2	54
7	Searching for the Hidden Hydrides: The Competition between Alkene Isomerization and Metathesis with Grubbs Catalysts. European Journal of Organic Chemistry, 2012, 2012, 5673-5677.	2.4	41
8	Quantifying Electron Correlation of the Chemical Bond. Journal of Physical Chemistry Letters, 2017, 8, 1937-1942.	4.6	41
9	Understanding the Decomposition Pathways of Mixed Sulfur/Selenium Lead Phosphinato Complexes Explaining the Formation of Lead Selenide. Journal of Physical Chemistry C, 2011, 115, 16904-16909.	3.1	37
10	The Mechanism of the Stereospecific Intramolecular Arylation of Lithiated Ureas: The Role of Li⁺ Probed by Electronic Structure Calculations, and by NMR and IR Spectroscopy. European Journal of Organic Chemistry, 2012, 2012, 731-743.	2.4	35
11	A DFT study of the possible role of vinylidene and carbene intermediates in the mechanism of the enzyme acetylene hydratase. Dalton Transactions, 2010, 39, 3816.	3.3	33
12	Binding Energy of F(H2O)- and the Simulation of Fluoride Water Clusters Using a Hybrid QM/MM (Fluctuating Charge) Potential. Journal of Physical Chemistry A, 1999, 103, 4094-4100.	2.5	31
13	The structure and interaction energies of the weak complexes of CHClF2 and CHF3 with HCCH: a test of density functional theory methods. Physical Chemistry Chemical Physics, 2011, 13, 4388.	2.8	31
14	Speciation in Aqueous Zinc Chloride. Anab InitioHybrid Microsolvation/Continuum Approach. The Journal of Physical Chemistry, 1996, 100, 9689-9693.	2.9	30
15	Machine Learning of Dynamic Electron Correlation Energies from Topological Atoms. Journal of Chemical Theory and Computation, 2018, 14, 216-224.	5.3	29
16	The potential energy surfaces of N2O2 species: implications for selective catalytic reduction. Physical Chemistry Chemical Physics, 2000, 2, 707-714.	2.8	28
17	Accurate Prediction of Adsorption Energies on Graphene, Using a Dispersion-Corrected Semiempirical Method Including Solvation. Journal of Chemical Information and Modeling, 2014, 54, 2255-2260.	5.4	27
18	Exploration of the Mechanism of the Oxidation of Sulfur Dioxide and Bisulfite by Hydrogen Peroxide in Water Clusters UsingAb InitioMethods. Journal of the American Chemical Society, 1998, 120, 3431-3439.	13.7	26

#	Article	IF	Citations
19	Lithium Choreography Determines Contrasting Stereochemical Outcomes of Aryl Migrations in Benzylic Carbamates, Ureas and Thiocarbamates. European Journal of Organic Chemistry, 2015, 2015, 953-959.	2.4	26
20	The solvated fluoride anion can be a good nucleophile. Chemical Communications, 2005, , 5902.	4.1	22
21	The structure and binding energies of the van der Waals complexes of Ar and N2 with phenol and its cation, studied by high level ab initio and density functional theory calculations. Journal of Chemical Physics, 2008, 128, 044313.	3.0	22
22	Cadmium Sulfide and Cadmium Phosphide Thin Films from a Single Cadmium Compound. Inorganic Chemistry, 2011, 50, 2052-2054.	4.0	22
23	Initial Studies Directed toward the Rational Design of Aqueous Graphene Dispersants. ACS Omega, 2019, 4, 1969-1981.	3.5	14
24	Stereospecificity in Reactions of Allylstannanes with Aldehydes Explored by Electronic Structure Calculations. Journal of Organic Chemistry, 1999, 64, 4680-4684.	3.2	13
25	The effects of higher orders of perturbation theory on the correlation energy of atoms and bonds in molecules. International Journal of Quantum Chemistry, 2018, 118, e25519.	2.0	13
26	Do Nitrogen-Containing Oxocarbons Exist? Predictions of Their Stability and Aromaticity. Journal of Physical Chemistry A, 2001, 105, 10689-10693.	2.5	9
27	Aerosol-assisted CVD of cadmium diselenoimidodiphosphinate and formation of a new iPr2N2P3+ ion supported by combined DFT and mass spectrometric studies. Dalton Transactions, 2016, 45, 18603-18609.	3.3	9
28	A Comparison of the Interacting Quantum Atoms (IQA) Analysis of the Twoâ€Particle Densityâ€Matrices of MP4SDQ and CCSD. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2020, 646, 1244-1251.	1.2	8
29	The deposition of cadmium selenide and cadmium phosphide thin films from cadmium thioselenoimidodiphosphinate by AACVD and the formation of an aromatic species. Dalton Transactions, 2019, 48, 1436-1442.	3.3	7
30	Lithiated Tertiary Carbanions Display Variable Coordination Modes: Evidence from DFT and NMR Studies. Chemistry - A European Journal, 2012, 18, 11036-11045.	3.3	5
31	Modelling of Transition States in Condensed Phase Reactivity Studies. ACS Symposium Series, 1999, , 401-410.	0.5	1