Thomas A Manz

List of Publications by Year
in descending order

34	2,618	489802 18	406436 35
papers	citations	h-index	g-index

37	37	37	2276
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Parametrization of Nonbonded Force Field Terms for Metalâ€“Organic Frameworks Using Machine Learning Approach. Journal of Chemical Information and Modeling, 2021, 61, 5774-5784.	2.5	5
2	Identifying misbonded atoms in the 2019 CoRE metalâ€“organic framework database. RSC Advances, 2020, 10, 26944-26951.	1.7	22
3	Seven confluence principles: a case study of standardized statistical analysis for 26 methods that assign net atomic charges in molecules. RSC Advances, 2020, 10, 44121-44148.	1.7	14
4	New scaling relations to compute atom-in-material polarizabilities and dispersion coefficients: part 1. Theory and accuracy. RSC Advances, 2019, 9, 19297-19324.	1.7	16
5	Bond orders of the diatomic molecules. RSC Advances, 2019, 9, 17072-17092.	1.7	18
6	New scaling relations to compute atom-in-material polarizabilities and dispersion coefficients: part 2. Linear-scaling computational algorithms and parallelization. RSC Advances, 2019, 9, 33310-33336.	1.7	10
7	A collection of forcefield precursors for metalâ€“organic frameworks. RSC Advances, 2019, 9, 36492-36507.	1.7	21
8	Introducing DDEC6 atomic population analysis: part 4. Efficient parallel computation of net atomic charges, atomic spin moments, bond orders, and more. RSC Advances, 2018, 8, 2678-2707.	1.7	129
9	Professional Communication, 2018, 61, 221-222.	0.6	0
10	Synthesis and Characterization of N,Nâ€²-Bismesityl Phenanthrene-9,10-diimine and Imineâ€“Nitrone. ACS Omega, 2018, 3, 16858-16865.	1.6	1
11	Introducing DDEC6 atomic population analysis: part 3. Comprehensive method to compute bond orders. RSC Advances, 2017, 7, 45552-45581.	1.7	327
12	Computationally designed tandem direct selective oxidation using molecular oxygen as oxidant without coreductant. RSC Advances, 2016, 6, 88189-88215.	1.7	2
13	Introducing DDEC6 atomic population analysis: part 2. Computed results for a wide range of periodic and nonperiodic materials. RSC Advances, 2016, 6, 45727-45747.	1.7	351
14	Introducing DDEC6 atomic population analysis: part 1. Charge partitioning theory and methodology. RSC Advances, 2016, 6, 47771-47801.	1.7	567
15	Computationally designed zirconium organometallic catalyst for direct epoxidation of alkenes without allylic H atoms: aromatic linkage eliminates formation of inert octahedral complexes. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	3
16	Hafnium catalysts for direct alkene epoxidation using molecular oxygen as oxidant. RSC Advances, 2015, 5, 12311-12322.	1.7	6
17	Deactivation of Ti and Zr half-metallocene complexes activated with B(C₆F₅)₃: a case study in constructing DFT-based QSARs to predict unimolecular rate constants. RSC Advances, 2015, 5, 48246-48254.	1.7	12
18	Expanding the Scope of Density Derived Electrostatic and Chemical Charge Partitioning to Thousands of Atoms. Journal of Chemical Theory and Computation, 2014, 10, 5377-5390.	2.3	32

#	Article	IF	Citations
19	Selective oxidation passing through Î·³-ozone intermediates: applications to direct propene epoxidation using molecular oxygen oxidant. RSC Advances, 2014, 4, 27755-27774.	1.7	12
20	Synthesis, Characterization, and Computation of Catalysts at the Center for Atomic-Level Catalyst Design. Journal of Physical Chemistry C, 2014, 118, 20043-20069.	1.5	21
21	Effects of electrostatic interactions on gas adsorption and permeability of MOF membranes. Molecular Simulation, 2014, 40, 557-570.	0.9	22
22	Near Surface Phase Transition of Solute Derived Pt Monolayers. Topics in Catalysis, 2013, 56, 1065-1073.	1.3	8
23	Computing Accurate Net Atomic Charges, Atomic Spin Moments, and Effective Bond Orders in Complex Materials. RSC Catalysis Series, 2013, , 192-222.	0.1	2
24	Comment on â€œExtending Hirshfeldâ€‰ to bulk and periodic materialsâ€•. Journal of Computational Chemistry, 2013, 34, 418-421.	1.5	6
25	Antiphase domain boundaries at the Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>(001) surface. Physical Review B, 2012, 85, .	1.1	37
26	Improved Atoms-in-Molecule Charge Partitioning Functional for Simultaneously Reproducing the Electrostatic Potential and Chemical States in Periodic and Nonperiodic Materials. Journal of Chemical Theory and Computation, 2012, 8, 2844-2867.	2.3	282
27	Structureâ€“Activity Correlation for Relative Chain Initiation to Propagation Rates in Single-Site Olefin Polymerization Catalysis. Organometallics, 2012, 31, 602-618.	1.1	20
28	Accurate Treatment of Electrostatics during Molecular Adsorption in Nanoporous Crystals without Assigning Point Charges to Framework Atoms. Journal of Physical Chemistry C, 2011, 115, 4824-4836.	1.5	106
29	Methods for Computing Accurate Atomic Spin Moments for Collinear and Noncollinear Magnetism in Periodic and Nonperiodic Materials. Journal of Chemical Theory and Computation, 2011, 7, 4146-4164.	2.3	77
30	A dimensionless reaction coordinate for quantifying the lateness of transition states. Journal of Computational Chemistry, 2010, 31, 1528-1541.	1.5	11
31	Chemically Meaningful Atomic Charges That Reproduce the Electrostatic Potential in Periodic and Nonperiodic Materials. Journal of Chemical Theory and Computation, 2010, 6, 2455-2468.	2.3	365
32	Quantitative Effects of Ion Pairing and Sterics on Chain Propagation Kinetics for 1-Hexene Polymerization Catalyzed by Mixed Cpâ€²/ArO Complexes. Organometallics, 2008, 27, 5504-5520.	1.1	25
33	Structureâ”Activity Correlation in Titanium Single-Site Olefin Polymerization Catalysts Containing Mixed Cyclopentadienyl/Aryloxide Ligation. Journal of the American Chemical Society, 2007, 129, 3776-3777.	6.6	51
34	The nature of aryloxide and arylsulfide ligand bonding in dimethyltitanium complexes containing cyclopentadienyl ligation. Dalton Transactions, 2005, , 668.	1.6	14