Thomas A Manz

List of Publications by Year
in descending order

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34 papers	2,618 citations	430874 18 h-index	361022 35 g-index
37 all docs	37 docs citations	37 times ranked	2005 citing authors

#	Article	IF	Citations
1	Introducing DDEC6 atomic population analysis: part 1. Charge partitioning theory and methodology. RSC Advances, 2016, 6, 47771-47801.	3.6	567
2	Chemically Meaningful Atomic Charges That Reproduce the Electrostatic Potential in Periodic and Nonperiodic Materials. Journal of Chemical Theory and Computation, 2010, 6, 2455-2468.	5.3	365
3	Introducing DDEC6 atomic population analysis: part 2. Computed results for a wide range of periodic and nonperiodic materials. RSC Advances, 2016, 6, 45727-45747.	3.6	351
4	Introducing DDEC6 atomic population analysis: part 3. Comprehensive method to compute bond orders. RSC Advances, 2017, 7, 45552-45581.	3.6	327
5	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.	5.3	282
6	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.	3.6	129
7	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.	3.1	106
8	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.	5.3	77
9	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.	13.7	51
10	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, .	3.2	37
11	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.	5.3	32
12	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.	2.3	25
13	Effects of electrostatic interactions on gas adsorption and permeability of MOF membranes. Molecular Simulation, 2014, 40, 557-570.	2.0	22
14	Identifying misbonded atoms in the 2019 CoRE metalâ€“organic framework database. RSC Advances, 2020, 10, 26944-26951.	3.6	22
15	Synthesis, Characterization, and Computation of Catalysts at the Center for Atomic-Level Catalyst Design. Journal of Physical Chemistry C, 2014, 118, 20043-20069.	3.1	21
16	A collection of forcefield precursors for metalâ€“organic frameworks. RSC Advances, 2019, 9, 36492-36507.	3.6	21
17	Structureâ€“Activity Correlation for Relative Chain Initiation to Propagation Rates in Single-Site Olefin Polymerization Catalysis. Organometallics, 2012, 31, 602-618.	2.3	20
18	Bond orders of the diatomic molecules. RSC Advances, 2019, 9, 17072-17092.	3.6	18

#	Article	IF	Citations
19	New scaling relations to compute atom-in-material polarizabilities and dispersion coefficients: part 1. Theory and accuracy. RSC Advances, 2019, 9, 19297-19324.	3.6	16
20	The nature of aryloxide and arylsulfide ligand bonding in dimethyltitanium complexes containing cyclopentadienyl ligation. Dalton Transactions, 2005, , 668.	3.3	14
21	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.	3.6	14
22	Selective oxidation passing through Î·³-ozone intermediates: applications to direct propene epoxidation using molecular oxygen oxidant. RSC Advances, 2014, 4, 27755-27774.	3.6	12
23	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.	3.6	12
24	A dimensionless reaction coordinate for quantifying the lateness of transition states. Journal of Computational Chemistry, 2010, 31, 1528-1541.	3.3	11
25	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.	3.6	10
26	Near Surface Phase Transition of Solute Derived Pt Monolayers. Topics in Catalysis, 2013, 56, 1065-1073.	2.8	8
27	Comment on â€œExtending Hirshfeldâ€¦ to bulk and periodic materialsâ€•. Journal of Computational Chemistry, 2013, 34, 418-421.	3.3	6
28	Hafnium catalysts for direct alkene epoxidation using molecular oxygen as oxidant. RSC Advances, 2015, 5, 12311-12322.	3.6	6
29	Parametrization of Nonbonded Force Field Terms for Metalâ€“Organic Frameworks Using Machine Learning Approach. Journal of Chemical Information and Modeling, 2021, 61, 5774-5784.	5.4	5
30	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.	1.4	3
31	Computing Accurate Net Atomic Charges, Atomic Spin Moments, and Effective Bond Orders in Complex Materials. RSC Catalysis Series, 2013, , 192-222.	0.1	2
32	Computationally designed tandem direct selective oxidation using molecular oxygen as oxidant without coreductant. RSC Advances, 2016, 6, 88189-88215.	3.6	2
33	Synthesis and Characterization of N,Nâ€²-Bismesityl Phenanthrene-9,10-diimine and Imineâ€“Nitrone. ACS Omega, 2018, 3, 16858-16865.	3.5	1
34	Professional Communication, 2018, 61, 221-222.	0.8	0