Xin Wu

List of Publications by Year in descending order

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13 papers	1,077 citations	687363 13 h-index	996975 15 g-index
17 all docs	17 docs citations	17 times ranked	890 citing authors

#	Article	IF	Citations
1	Isolation and Characterization of Sc2C2@C68: A Metal-Carbide Endofullerene with a Non-IPR Carbon Cage. Angewandte Chemie - International Edition, 2006, 45, 2107-2111.	13.8	181
2	Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Theory, Implementation, and Parameters. Journal of Chemical Theory and Computation, 2016, 12, 1082-1096.	5.3	123
3	Crystal Structures of Saturnâ€Like C₅₀Cl₁₀ and Pineappleâ€Shaped C₆₄Cl₄: Geometric Implications of Doubleâ€and Tripleâ€Pentagonâ€Fused Chlorofullerenes. Angewandte Chemie - International Edition, 2008, 47, 5340-5343.	13.8	116
4	Two Ih-symmetry-breaking C60 isomers stabilized by chlorination. Nature Materials, 2008, 7, 790-794.	27.5	114
5	Dimetalloendofullerene U2@C60Has a Uâ‹U Multiple Bond Consisting of Sixfold One-Electron-Two-Center Bonds. Journal of the American Chemical Society, 2007, 129, 2171-2177.	13.7	95
6	Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Benchmarks for Ground-State Properties. Journal of Chemical Theory and Computation, 2016, 12, 1097-1120.	5.3	74
7	An Entrant of Smaller Fullerene: C56 Captured by Chlorines and Aligned in Linear Chains. Journal of the American Chemical Society, 2008, 130, 15240-15241.	13.7	69
8	Hybrid Quantum and Classical Simulations of the Dihydrofolate Reductase Catalyzed Hydride Transfer Reaction on an Accurate Semi-Empirical Potential Energy Surface. Journal of Chemical Theory and Computation, 2011, 7, 3420-3437.	5.3	45
9	Semiempirical Quantum-Chemical Methods with Orthogonalization and Dispersion Corrections. Journal of Chemical Theory and Computation, 2019, 15, 1743-1760.	5.3	45
10	Semiempirical Quantum Chemical Calculations Accelerated on a Hybrid Multicore CPUâ€“GPU Computing Platform. Journal of Chemical Theory and Computation, 2012, 8, 2272-2281.	5.3	44
11	Specific Reaction Path Hamiltonian for Proton Transfer in Water: Reparameterized Semiempirical Models. Journal of Chemical Theory and Computation, 2013, 9, 2672-2686.	5.3	42
12	Big data analysis of ab Initio molecular integrals in the neglect of diatomic differential overlap approximation. Journal of Computational Chemistry, 2019, 40, 638-649.	3.3	10
13	Structures and Electronic Properties of M2C2 @C78(M = Ti, Zr, Hf): A Density Functional Theory Study. Journal of Nanoscience and Nanotechnology, 2007, 7, 1346-1352.	0.9	8