# Thomas Weymuth

## List of Publications by Citations



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|---|---|---|---|
| 17 papers | 409 citations | 10 h-index | 20 g-index |
| 20 ext. papers | 468 ext. citations | 4.5 avg, IF | 3.89 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 17 | New Benchmark Set of Transition-Metal Coordination Reactions for the Assessment of Density Functionals. *Journal of Chemical Theory and Computation*, **2014**, 10, 3092-103 | 6.4 | 142 |
| 16 | M(O)V(I)P(AC): vibrational spectroscopy with a robust meta-program for massively parallel standard and inverse calculations. *Journal of Computational Chemistry*, **2012**, 33, 2186-98 | 3.5 | 50 |
| 15 | A local-mode model for understanding the dependence of the extended amide III vibrations on protein secondary structure. *Journal of Physical Chemistry B*, **2010**, 114, 10649-60 | 3.4 | 44 |
| 14 | Inverse quantum chemistry: Concepts and strategies for rational compound design. *International Journal of Quantum Chemistry*, **2014**, 114, 823-837 | 2.1 | 42 |
| 13 | Gradient-driven molecule construction: An inverse approach applied to the design of small-molecule fixating catalysts. *International Journal of Quantum Chemistry*, **2014**, 114, 838-850 | 2.1 | 24 |
| 12 | Characteristic Raman optical activity signatures of protein β-sheets. *Journal of Physical Chemistry B*, **2013**, 117, 11943-53 | 3.4 | 23 |
| 11 | Redox-Active Chiroptical Switching in Mono- and Bis-Iron Ethynylcarbo[6]helicenes Studied by Electronic and Vibrational Circular Dichroism and Resonance Raman Optical Activity. *Chemistry - A European Journal*, **2018**, 24, 15067-15079 | 4.8 | 19 |
| 10 | Statistical Analysis of Semiclassical Dispersion Corrections. *Journal of Chemical Theory and Computation*, **2018**, 14, 2480-2494 | 6.4 | 18 |
| 9 | Identifying protein β-turns with vibrational Raman optical activity. *ChemPhysChem*, **2011**, 12, 1165-75 | 3.2 | 13 |
| 8 | How many chiral centers can Raman optical activity spectroscopy distinguish in a molecule?. *Journal of Physical Chemistry A*, **2012**, 116, 5410-9 | 2.8 | 10 |
| 7 | Systematic dependence of transition-metal coordination energies on density-functional parametrizations. *International Journal of Quantum Chemistry*, **2015**, 115, 90-98 | 2.1 | 6 |
| 6 | Expansive Quantum Mechanical Exploration of Chemical Reaction Paths.. *Accounts of Chemical Research*, **2021**, | 24.3 | 5 |
| 5 | Immersive Interactive Quantum Mechanics for Teaching and Learning Chemistry. *Chimia*, **2021**, 75, 45-49 | 1.3 | 5 |
| 4 | Toward an Inverse Approach for the Design of Small-Molecule Fixating Catalysts. *Materials Research Society Symposia Proceedings*, **2013**, 1524, 101 | | 4 |
| 3 | Density Functional Theory for Transition Metal Chemistry: The Case of a Water-Splitting Ruthenium Cluster **2011**, 137-163 | | 2 |
| 2 | Resonance Effects in the Raman Optical Activity Spectrum of [Rh(en)]. *Journal of Physical Chemistry A*, **2019**, 123, 9357-9370 | 2.8 | 1 |
| 1 | The Transferability Limits of Static Benchmarks. *Physical Chemistry Chemical Physics*, | 3.6 | 1 |