

# Matthew D Kundrat

## List of Publications by Year in descending order

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8  
papers

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1307594  
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citing authors

#	ARTICLE	IF	CITATIONS
1	Hydrogen Desorption Exceeding Ten Weight Percent from the New Quaternary Hydride Li <sub>3</sub> BN <sub>2</sub> H <sub>8</sub> . Journal of Physical Chemistry B, 2005, 109, 6-8.	2.6	307
2	Calculation of circular dichroism spectra from optical rotatory dispersion, and vice versa, as complementary tools for theoretical studies of optical activity using time-dependent density functional theory. Journal of Chemical Physics, 2006, 125, 194110.	3.0	57
3	Time Dependent Density Functional Theory Modeling of Chiroptical Properties of Small Amino Acids in Solution. Journal of Physical Chemistry A, 2006, 110, 4115-4123.	2.5	47
4	Ab Initio and Density Functional Theory Modeling of the Chiroptical Response of Glycine and Alanine in Solution Using Explicit Solvation and Molecular Dynamics. Journal of Chemical Theory and Computation, 2008, 4, 1902-1914.	5.3	47
5	Modeling of the Chiroptical Response of Chiral Amino Acids in Solution Using Explicit Solvation and Molecular Dynamics. Journal of Chemical Theory and Computation, 2009, 5, 1051-1060.	5.3	46
6	Computational Modeling of the Optical Rotation of Amino Acids: A New Look at an Old Rule for pH Dependence of Optical Rotation. Journal of the American Chemical Society, 2008, 130, 4404-4414.	13.7	38
7	Time Dependent Density Functional Theory Modeling of Specific Rotation and Optical Rotatory Dispersion of the Aromatic Amino Acids in Solution. Journal of Physical Chemistry A, 2006, 110, 12908-12917.	2.5	30
8	Hydrogen Desorption Exceeding Ten Weight Percent from the New Quaternary Hydride Li <sub>3</sub> BN <sub>2</sub> H <sub>8</sub> . ChemInform, 2005, 36, no.	0.0	2