

**Application of the Time-Dependent Density  
Functional Theory to the Study of  
Chiroptical Properties of Organic and  
Inorganic Compounds**

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vorgelegte Dissertation

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**Yuekui Wang**

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*My wife, Yuanlin Di, and  
my daughter, Shuo Wang.*

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# List of Publications

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1. G. Raabe, C. Repges, Y. Wang, and J. Fleischhauer, *Enantiomer*, 2002, **7** (2–3), 77–83.

*Determination of the Absolute Configuration of Rubroflavin by Comparison of Measured and Calculated CD Spectra of its Thermolysis Product 3-Methanesulfinyl-5-Methylmercaptophenol.*

2. Y. Wang, J. Fleischhauer, S. Bausch, M. Sebastian, and P. H. Laur, *Enantiomer*, 2002, **7** (6), 343–374.

*Conformational Analysis and TDDFT Calculations of the Chiroptical Properties of Tris[1,2-propanediolato(2-)-κO,κO']selenium/tellurium and Related Compounds.*

3. Y. Wang, G. Raabe, C. Repges, and J. Fleischhauer, *Int. J. Quan. Chem.*, 2003, **93** (4), 265–270.

*Time -Dependent Density Functional Theory (TDDFT) Calculations on the Chiroptical Properties of Rubroflavin. Determination of its Absolute Configuration by Comparison of Measured and Calculated CD Spectra.*