Personal Details

Name	Matthew D. Kundrat, PhD
Date of birth	26 February 1976
Place of birth	Pittsburgh, PA, USA
Nationality	American
Marital Status:	Single
Address	Kaiserstraße 22
	76133 Karlsruhe, Germany
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PhD in Computational Chemistry, MA in Inorganic Chemistry

6 years experience in computational chemistry / molecular modeling
3 years experience in scientific marketing / webpage development
5 years experience in experimental (air sensitive) inorganic and analytical chemistry
7 years experience in teaching general, inorganic and physical chemistry

Career History

- July 2012..July 2014 Post-doc, Karlsruher Institut für Technologie – Karlsruhe, GER
Primary project involved modeling of charge transfer systems using Partition Density Functional Theory. Also collaborated on projects where I modelled the results of Kelvin probe force microscopy, as well as X-ray emission and absorption. Programs used included ADF, Turbomole, ORCA, and GROMACS.

- Feb 2009..Dec 2011 Staff Scientist, Scientific Computing and Modelling – Amsterdam, NED
In charge of marketing, webpage development, documentation, support and promotion of the Amsterdam Density Functional suite of programs for molecular modeling. Represented the company at many international chemistry and physics conferences, including the ACS, APS, ICQC, WATOC, and DFT exhibitions. Also gave presentations and hosted software workshops at universities, government research centers and private businesses throughout the US and Europe.

- Aug 2004..Dec 2008 Research / Teaching Assistant, SUNY at Buffalo – Amherst, NY
Modeled chiroptical properties of amino acids in solution using time dependent density functional theory. Compared computed specific rotation, optical rotatory dispersion and circular dichroism to experimental values. Solvation effects were modeled with the COSMO continuum model as well as explicitly through the direct reaction field method. Software used included Turbomole, ADF, Gaussian03, DRF-90, GROMACS, gOpenMol and Molden, all running under Linux. Teaching duties included general chemistry for engineers: recitation and laboratories.

- Sept 2001..Sept 2003 Chemist, General Motors R&D – Warren, MI
Synthesized and evaluated the performance of air-sensitive metal hydrides designed as potential hydrogen fuel storage compounds for automobiles. Also served as X-ray crystallographer, performing phase identification and particle size analysis on various metals, alloys and metal-coated materials.

- July 2001..Sept 2001 Paint Quality Technician, PPG – Warren, MI
Monitored quality of paint coatings on 2002 Dodge trucks at the Daimler-Chrysler assembly plant. Helped to identify and fix flaws in the painting process, reducing the number of vehicles rejected due to paint defects.

- Sept 2000..Dec 2000 Adj. Prof. of Inor. Chem., University of Mich., Dearborn – Dearborn, MI
Instructed students in advanced inorganic laboratory. Was responsible for deciding the curriculum, setting up the laboratory, supervising the experiments and assigning grades.

- Aug 1997..Dec 2000 Research / Teaching Assistant, Wayne State University – Detroit, MI
Designed and synthesized novel precursors for the chemical vapor deposition of gallium antimodide as well as titanium and tantalum nitrides. The projects emphasized synthetic and analytical work, utilizing standard glove-box and Schlenk-line techniques for handling air-sensitive materials and using IR, NMR, MS, EA, and X-ray crystallography to characterize products. My synthetic work was strongly supplemented with ab-initio computational analyses of model compounds using Gaussian 98.
Teaching duties included general chemistry quiz sessions and laboratories for science and engineering students, as well as inorganic chemistry laboratory.

- Sept 1994..May 1997 Laboratory Assistant, Clarion University of Pennsylvania – Clarion, PA
Supervised the setup and cleanup of the reagents and equipment essential for the completion of general and organic chemistry laboratories. Managed junior lab assistants in these tasks. Provided further assistance to the professors and students during the class periods.

Education

- 2008 Ph.D. in Computational Chemistry GPA: 3.84 / 4.00
State University of New York at Buffalo

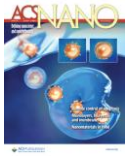
- 2004 M.A. in Inorganic Chemistry
Wayne State University

- 1997 B.S. in Chemistry with a minor in Computer Science
Clarion University of Pennsylvania

Certifications / Trainings / Achievements / Awards / Languages / Computer Programming

2012-2015	German as a foreign language, intermediate ~B1
2009-2011	Dutch as a foreign language, advanced beginner ~A2
1997	Clarion University Chemistry Department Competitive Award
1994	Advanced Placement Scholar with Distinction
1994-2015	Computer programming in Pascal, Assembly, C, shell scripts (bash), HTML

Publications

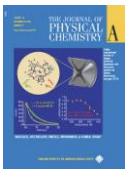


11. Neff, Julia L.; Milde, Peter; Pérez León, Carmen; Kundrat, Matthew D.; Eng, Lukas M.; Jacob, Christoph R.; Hoffmann-Vogel, Regina. Epitaxial growth of pentacene on alkali halide surfaces studied by kelvin probe force microscopy. ACS Nano; **2014**; *8*(4) pp 3294-3301.

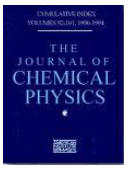
10. Kundrat, Matthew D.; Autschbach, Jochen. Modeling of the chiroptical response of chiral amino acids in solution using explicit solvation and molecular dynamics. Journal of Chemical Theory and Computation; **2009**; 5 (4) pp 1051-1060.

9. Kundrat, Matthew D.; Autschbach, Jochen. 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*(11) pp 1902-1914.

8. Kundrat, Matthew D.; Autschbach, Jochen. 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*(13) pp 4004-4414.

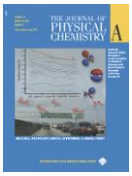


7. Kundrat, Matthew D.; Autschbach, Jochen. Time dependent density functional theory modeling of specific rotation and optical rotatory dispersion of the aromatic amino acids in solution. Journal of Physical Chemistry A; **2006**; *110*(47) pp 12908-12917.



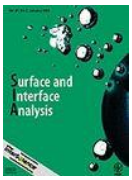
6. Krykunov, Mykhaylo; Kundrat, Matthew D.; Autschbach, Jochen. Calculation of CD spectra from optical rotatory dispersion, and vice versa, as complementary tools for theoretical studies of optical activity using time-dependent density functional theory. Journal of Chemical Physics; **2006**; *125* pp 194110-194122.

5.Balogh, Michael P.; Jones, Camille Y.; Herbst, J.F.; Hector, Jr., Louis G.; Kundrat, Matthew. Crystal structures and phase transformation of deuterated lithium imide, Li_2ND. Journal of Alloys and Compounds; **2006;** *420* pp 326-336.



4. Kundrat, Matthew D.; Autschbach, Jochen. Time dependent density functional theory modeling of chiroptical properties of small amino acids in solution. Journal of Physical Chemistry A; **2006**; *110*(11) pp 4115-4123.

3. Meisner, Gregory P.; Pinkerton, Frederick E.; Meyer, Martin S.; Balogh, Michael P.; Kundrat, Matthew D.. Study of the lithium-nitrogen-hydrogen system. Journal of Alloys and Compounds; **2005**; *404-406* pp 24-26.



2. Gaarenstroom, Stephen W.; Balogh, Michael P.; Militello, Maria C.; Waldo, Richard A.; Wong, Curtis A.; Kelly, Nelson A.; Gibson, Thomas L.; Kundrat, Matthew D.. Characterization of indium-tin-oxide films with improved corrosion resistance. Surface and Interface Analysis **2005**; *37*(4), pp 385-392.

1. Pinkerton, Frederick E.; Meisner, Gregory P.; Meyer, Martin S.; Balogh, Michael P.; Kundrat, Matthew D.. Hydrogen desorption exceeding ten weight percent from the new quaternary hydride $Li_3BN_2H_8$ Journal of Physical Chemistry B; **2005**; *109*(1) pp 6 - 8.

Selected Conference Participation

8. Kundrat, Matthew D.; Atkins, Andrew J.; Jacob, Christoph R.. Modeling solvent effects on X-ray Spectroscopy. Poster presented at the 10th Congress of the World Association of Theoretical and Computational Chemists , Santiago, Chile, October 5-10 2014, and at the 50th Symposium on Theoretical Chemistry, Vienna, Austria, September 14-18 2014

7. Kundrat, Matthew D.; Jacob, Christoph. R. Towards the description of ground-state charge transfer at organic interfaces with subsystem-DFT. Poster presented at the 15th International Conference on Density Functional Theory and its Applications , Durham, UK, September 9-13 2013, and at the 49th Symposium on Theoretical Chemistry, Erlangen, Germany, September 22-26 2013.

6. Kundrat, Matthew D.; Autschbach, Jochen. Modeling the effects of an achiral solvent on the chiroptical response properties of chiral amino acids. Talk presented at 40th Midwest Theoretical Chemistry Conference, Ann Arbor, MI, June 26-28 2008.

5. Kundrat, Matthew D.; Autschbach, Jochen. Time-dependent density functional theory calculation of specific rotation using molecular dynamics and explicit solvation. Poster *and* talk presented at 233rd ACS National Meeting, Chicago, IL, March 25-29, 2007; PHYS 566.

4. Kundrat, Matthew D.; Autschbach, Jochen. Specific rotation of amino acids: A new look at an old rule. Poster presented at 232nd ACS National Meeting, San Francisco, CA, Sept. 10-14, 2006, PHYS 449.

3. Kundrat, Matthew D.; Autschbach, Jochen. Time-dependent density functional theory modeling of the chiroptical properties of aromatic amino acids in solution. Poster presented at 38th Midwest Theoretical Chemistry Conference, Columbus, OH, June 15-17, 2006.

2. Kundrat, Matthew D.; Autschbach, Jochen. Comparison of methods of density functional theory modeling of the specific rotation of amino acid solutions. Poster presented at 230th ACS National Meeting, Washington, DC, Aug. 28-Sept. 1, 2005, COMP 215.

1. Second Annual Wayne State University Graduate Research Symposium: Organizing committee member. Detroit, MI, August 18, 2000.

Patents

2. Meisner, Gregory P.; Pinkerton, Frederick E.; Meyer, Martin S.; Balogh, Michael P.; Kundrat, Matthew D.. Imide/amide hydrogen storage materials and methods. United States Patent #7344690, Mar. 18, 2008.

1. Meisner, Gregory P.; Pinkerton, Frederick E.; Meyer, Martin S.; Balogh, Michael P.; Kundrat, Matthew D.. Imide/amide hydrogen storage materials and methods. United States Patent #6967012, Nov. 22, 2005.

An up-to-date version of this resume, along with my PhD thesis and links to publications can be found at my website at: http://mattkundrat.eu