

# Matthew D. Kundrat, PhD

## PhD in Physical Chemistry, MA in Inorganic Chemistry, minor in Computer Science

*A research scientist with over 20 years of professional experience*

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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

**Environmental Chemist II**, [PA Department of Environmental Protection](#) – Harrisburg, PA; Oct 2016-present

- Developed standards for the legal limits of pollutants discharged into waterways, including common ions, metals and synthetic toxins
- Collaborated with other scientists as well as engineers, lawyers and political appointees to ensure that the standards enacted are scientifically sound, legally defensible and practically applicable

**Scientist**, [Wilshire Technologies](#) – Princeton, NJ; Sept 2016

- Prepared marketing materials and price quotes for the sale of cGMP grade (current good manufacturing practice), vegetal and animal derived reagents for the synthesis of cosmetics and pharmaceuticals

**Research Scientist**, [Karlsruher Institut für Technologie](#) – Karlsruhe, GER; July 2012..July 2014

- Modeled charge transfer complexes using Partition Density Functional Theory and molecular dynamics, using the ADF, Turbomole, ORCA, and GROMACS programs and Python scripts
- Detailed the electronic characteristics of a molecular electronics system of adsorbed organic molecules on a metallic surface measured by Kelvin probe force microscopy
- Modeled plausible structures and X-ray emission and absorption spectra of heterogeneous catalysts

**Scientific Marketing Manager**, [Scientific Computing and Modelling](#) – Amsterdam, NED; Feb 2009..Dec 2011

- Represented the company at dozens of international chemistry and physics conferences, greeting, informing and gaining contact information from potential customers, causing a growth in revenues
- Presented PowerPoint seminars and hosted software workshops at universities, government research centers and private businesses, informing and educating current and potential customers
- Designed and distributed brochures, news items and press releases regarding the latest scientific innovations in software for molecular modeling
- Optimized company website using search engine optimization techniques with the aid of Google Analytics, employing standard HTML and CSS programming techniques, and ran online ad campaigns, increasing webpage hits by approximately 40%
- Provided customer support by e-mail, answering technical questions and relaying problem descriptions to our programming team

**Career History (continued)****Research / Teaching Assistant, [State University of New York at Buffalo](#)** – Amherst, NY; Aug 2004..Dec 2008

- Modeled chiroptical properties of amino acids in solution, including optical rotatory dispersion and circular dichroism, using time dependent density functional theory
- Utilized Turbomole, ADF, Gaussian03, DRF-90, GROMACS, gOpenMol and Molden molecular modeling software, running under Linux, Windows and Mac OS
- Presented my work at five national and regional conferences, and published an equal number of well-cited, peer-reviewed papers as principal author
- Instructed chemistry and chemical engineering students in quiz and laboratory sessions
- Mentored undergraduate students, helping them to begin their studies in theoretical chemistry

**Synthetic and Analytical Chemist, [General Motors Research and Development Center](#)** – Warren, MI; Sept 2001..Sept 2003

- Worked in a team of chemists, physicists and engineers to synthesize and evaluate the performance of air-sensitive metal hydrides designed as potential efficient, environmentally friendly hydrogen fuel storage compounds for automobiles
- Synthesized air-sensitive and moisture sensitive compounds using spray-drying and ball-milling for particle size control, all under an inert argon atmosphere
- Evaluated hydrogen storage compounds via Thermo Gravimetric Analysis (TGA) and real-time General Area Detector Diffraction System (GADDS) X-ray diffraction (XRD)
- Discovered a compound that yielded over 10% by weight desorbed hydrogen, leading to a groundbreaking publication which has been cited over 300 times to date
- Patented two inventions and published several papers and communications
- Analyzed both energy storage and catalytic systems by X-ray crystallography, performing phase identification and particle size analysis on various metals, alloys and metal-coated materials
- Communicated results to colleagues through our Lab Information Management Systems (LIMS)

**Paint Quality Technician, [PPG](#)** – Warren, MI; July 2001..Sept 2001

- Identified and fixed flaws in the painting process of Dodge trucks, increasing productivity and quality
- Enhanced consumer satisfaction by eliminating coating defects which caused customer complaints

**Adjunct Professor of Inorganic Chemistry, [University of Michigan, Dearborn](#)** – Dearborn, MI; Sept 2000..Dec 2000

- Instructed junior and senior level students in advanced inorganic laboratory
- Independently designed curriculum and graded performance of pupils
- Utilized pre-existing lab equipment and reagents extensively to conserve resources and stay under budget
- Managed laboratory insuring students completed complex experiments in a safe and timely manner

**Research / Teaching Assistant, [Wayne State University](#)** – Detroit, MI; Aug 1997..Dec 2000

- Designed and synthesized novel precursors for the chemical vapor deposition of the semiconductors gallium antimonide as well as titanium and tantalum nitrides, utilizing standard glove-box and Schlenk-line techniques for handling air-sensitive materials, with the aid of molecular modeling with ab-initio methods using the Gaussian 98 program
- Analyzed results using infrared spectroscopy (IR), nuclear magnetic resonance (NMR), mass spectrometry (MS), elemental analysis (EA), and X-ray crystallography to characterize products and verify their quality and purity
- Assisted professors in teaching general and inorganic chemistry to undergraduates

## Career History (continued)

**Analytical Laboratory Technician**, [Stewart Laboratories](#), Strattanville, PA July 1996..Aug 1996

- Tested soil samples for dioxin contamination utilizing supercritical fluid extraction methods coupled with gas chromatography / mass spectrometry (GCMS) in accord with the Environmental Protection Agency (EPA) and Pennsylvania Department of Environmental Protection (DEP) protocols
- Analyzed mine-drainage water and drinking water samples for metals, sulfates, non-dissolved solids, alkalinity and acidity, employing titration and gravimetric analysis techniques, ensuring standards for safety and quality were met

**Laboratory Assistant**, [Clarion University of Pennsylvania](#) – Clarion, PA; Sept 1994..May 1997

- Supervised the setup and cleanup of the reagents and equipment essential for the completion of general and organic chemistry laboratories, assisting professors and students during class period
- Oversaw two junior lab assistants in these tasks, setting goals and delegating tasks needed to keep 7 laboratories with 150 students running safely and efficiently

## Education

- Post-Doctoral Study in Computational Chemistry, Karlsruher Institut für Technologie, Karlsruhe, Germany
- Doctor of Philosophy in Computational Chemistry, State University of New York at Buffalo, GPA: 3.84 / 4.0, Dissertation title: “Time Dependent Density Functional Theory Modeling of Chiroptical Properties of Amino Acids in Solution”
- Master of Arts. in Inorganic Chemistry, Wayne State University, Detroit, MI
- Bachelor of Science in Chemistry with a minor in Computer Science, Clarion University of Pennsylvania, Clarion PA

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

- Foreign languages: Intermediate German (B1), Advanced Beginner Dutch (A2)
- Computer programming in Pascal, Assembly, C, shell scripts (bash), HTML
- 1997 Clarion University Chemistry Department Competitive Award
- 1994 Advanced Placement Scholar with Distinction, setting a new record for most credits earned by an incoming student at Clarion University

## Publications, Presentations and Patents

- Published [12 articles in peer reviewed journals](#), including the Journal of the American Chemical Society, the Journal of Physical Chemistry, the Journal of Chemical Theory and Computation, the Journal of Alloys and Compounds, Surface and Interface Analysis, The Journal of Chemical Physics, ACS Nano and Applied Surface Science
- Cited 690 times in total (h=11), with one paper cited over 300 times alone
- Patented twice for the invention of new hydrogen storage materials (US Patents [#7344960](#) and [#6967012](#))

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>