Dr. Peter Gedeck

Chemist · Computational and Physical Chemistry · German nationality
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Experience

2021-now Lecturer at University of Virginia School of Data Science

Teaching DS-6030 Statistical Learning and mentoring capstone projects

2018-now Research Informatics Senior Scientist at Collaborative Drug Discovery

Development of commercial cheminformatics and bioinformatics software for drug discovery.

- *CDD Vault*: Key contributions are development and implementation of AI functionality, extensions to the electronic lab notebook for ontology supported assay annotations and for synthesis planning using a stoichiometry table.
- *CDD PharmaKB*: Development of data offering product from concept to market introduction.
- *CDD BioAssay Express*: Work with customers from biotech and pharmaceutical companies to improve product.

Co-investigator on NIH (National Institutes of Health) and NLM (National Library of Medicine) supported Phase 1 to Phase 2B SBIR grants. Research areas include the development of novel approaches based on deep learning neural networks and other machine learning approaches.

Contribute to the scientific strategy of the research informatics and the product development group. Support sales efforts as needed. Mentor research informatics scientists and junior developers.

2018-2023 Instructor at Statistics.com

Instructor for *Predictive Analytics 1, 2, and 3 - Python.* The courses are offered three times a year. (https://www.statistics.com/dr-peter-gedeck)

Development of course material for three online courses: *Predictive Analytics 1, 2, and 3 - Python*. Co-author of the book *Data Mining for Business Analytics: Concepts, Techniques, and Applications in Python.* The book was published by John Wiley & Sons, Inc. in 2019 and forms the basis of the courses.

2017-now Owner at Peter Gedeck LLC

Development of novel cheminformatics approaches for drug discovery. Custom software development for scientific software companies.

Collaborative Drug Discovery: work on developing BioAssay Express from a research application to a product;

Cresset Biomolecular Discovery Ltd: implemented encrypted file format and adapted Blaze to use encrypted structural data at rest; develop PipelinePilot workflows for automatic alignment of larger datasets

Spring Global: develop and incorporate data science algorithms into their CPG software applications

2019-2022 Mentor and Advisor to ToxTrack, Inc.

Provide feedback on ToxTrack's business strategy, technical strategy, and development pipeline. Support business development efforts.

2018 Member of the IBM Watson Health - Drug Discovery Innovation Council

The objective of the council is to offer ideas and strategic guidance on IBM Watson Health's efforts to enable transformative innovation throughout the drug discovery process, leveraging the power of machine learning and cognitive computing.

1998-2016 Senior Investigator and Group Leader at Novartis

1998-2008: Novartis Institutes for BioMedical Research, Horsham, UK
2008-2012: Novartis Institutes for BioMedical Research, Basel, Switzerland
2012-2016: Novartis Institute for Tropical Diseases, Singapore, Singapore

Computational chemistry and cheminformatics support of research projects in respiratory, gastrointestinal, and tropical diseases. Activities covered target identification, hit finding and lead optimisation using structure and ligand based techniques.

Lead teams of computational chemists; responsible for budget, resourcing of research projects, performance management, and team development.

Initiated and supervised academic collaborations; mentored and supervised undergraduate and postgraduate students (NIBR presidential post doc, MSc students from the MSc Cheminformatics course of the University of Sheffield, and placement students from the University of Surrey).

Member of senior chemistry leadership team (Horsham, UK); contributed to strategic activities, advised on promotions and development of talent pool.

Member of Basel CADD leadership team. Responsibilities included project resourcing and developing the local CADD group, developing of global strategic activities, and extending and improving the software portfolio globally.

Leader of the GDC-IT Advisory Committee (July 2004 - June 2007). This team was responsible for monitoring and controlling chemistry related activities in the Novartis research IT organisation.

Represented research interests in the Novartis data warehouse project *Avalon*. Responsibilities included user requirements gathering, co-ordination of interaction between acceptance team and developers, discussion of design and functionality with development team, and testing of

pre-release versions. For this work, I was being awarded *The Novartis Business Partnership Award* together with the project team.

Lead a global team of seven computational chemists as part of the FOCUS project; responsible for developing the application, liaising with the vendor, and setting strategic directions. FOCUS is a scientific portal that integrates functionality for sharing, communicating, and analysing data, and designing new compounds. FOCUS enables the user to go from the analysis of disparate data to testing hypothesis to designing new compounds.

Core member of a cross-functional cheminformatics initiative. Objective was the development of a cheminformatics infrastructure and applications. Examples are: CIxFramework, infrastructure for model deployment with interfaces to FOCUS, Spotfire, and the Novartis data warehouse; HTS Explorer, a web application for interactive HTS data analysis and annotation; pKaCuration, platform for curating pKa datasets and training in house models; QSAR toolkit, predictive model development and deployment.

Evaluation of novel cheminformatics technology. Successfully introduced PipelinePilot (SciTegic) and FieldScreen (Cresset BioMolecular Discovery Ltd.) to Novartis.

1996-1998 Postdoctoral Fellow to Prof. Dr. T. Clark, Computer-Chemistry-Centre, Institute for Organic Chemistry I, University of Erlangen-Nürnberg, Germany

Postdoctoral Fellowship funded by Pfizer Ltd. Developed a QM/MM method for prediction of protein-ligand binding energies based on semiempirical molecular orbital calculations in cooperation with Pfizer Ltd. (Sandwich, UK).

Coordinated the development of the semiempirical molecular orbital program Vamp in cooperation with the Oxford Molecular Group (Oxford, UK); Vamp is now part of BIOVIA Materials Studio.

Participated in planning and organisation of the conference *Model(l)ing '97* (16th international meeting of the Molecular Graphics and Modelling Society MGMS, Erlangen, Germany, 2.-5. September 1997).

Supervised M.Sc. and Ph.D. students.

1991-1995 Research Assistant to Prof. Dr. S. Schneider, Institute for Physical Chemistry I, University of Erlangen-Nürnberg, Germany

Experimental and theoretical studies of intramolecular electron transfer in bridged donor-acceptor compounds. Quantum mechanical model calculations taking environmental solvent effects into account. Construction of a spectrometer for the measurement of fluorescence decay curves at low temperature.

Developed software for experiment control, data acquisition and data analysis.

Planned and administered the computer network of the Institutes of Physical and Theoretical Chemistry.

Supervised M.Sc. students. Conducted seminars and practicals.

Education

1998-2003 Fernuniversität Hagen, Germany (distance learning university). Introductory and advanced courses in mathematics, statistics and computer sciences.

1997-1998 University Erlangen-Nürnberg, Germany. Graduate college *Homogeneous and Heterogeneous Electron Transfer*.

1991-1995 University Erlangen-Nürnberg, Germany, Institute for Physical Chemistry I. Doctorate 26 January 1996 (Ph.D. thesis, *summa cum laude*), supervisor Prof. Dr. S. Schneider; *Doctoral fellowship* of the German Academic Scholarship Foundation.

1984-1991 University Erlangen-Nürnberg, Germany. Diploma in chemistry 6 November 1991 (Master thesis, *very good*), supervisor Prof. Dr. S. Schneider; *Fellowship* of the German Academic Scholarship Foundation.

1987-1988 Department of Chemistry, University College London, UK; *Fellowship* of the German Academic Exchange Service (DAAD).

Membership in Professional Organisations

2017-now Member of the *American Chemical Society* (ACS)

1998-2008 MRSC (Member) of the *Royal Society of Chemistry*

2001-2011 Committee member of the UK QSAR and Chemoinformatics Group. Redesigned and maintained the group's website. Organised two UK-QSAR group meetings in Horsham, UK (17th October 2001, 18th October 2006).

2004-2008 Ordinary committee member of the Molecular Graphics & Modelling Society (MGMS). On behalf of the MGMS, member of the organising committee of the 4th Joint Sheffield Conference on Chemoinformatics (Sheffield, UK, 18-20 June 2007).

Computer Skills

Scientific computing software:
Knowledgeable in the use of computational chemistry software (Biovia, Chemical Computing Group, Schrödinger, Cresset BioMolecular Discovery Ltd., Vamp, Mopac, Gaussian). Extensive experience with applications for data analysis and visualisation (R, scikit-learn, Spotfire)

Programming:
Design and development of procedural and object oriented programs using a wide variety of programming languages (Python, JavaScript, Java, Ruby, R, C++, Fortran, Pascal, Perl, VBasic). Design and development of web applications and web services using different technologies (Django, Ajax, React, JSP, REST)

Language Skills

German (mother tongue), English (fluent), French (intermediate)