R é s u m é

Dr. Axel Drefahl
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Chemist and Cheminformatician

Summary: Axel Drefahl is a chemist with work experiences in chemical software development, cheminformatics and clean-room operations in photovoltaic materials research. His research focuses on molecular modeling, design of algorithms for chemical property estimation, materials analysis and open-source software to encode complex chemical architectures and concepts (CurlySMILES).

Objective: Looking for new challenges in the rational design and characterization of advanced materials.

Interest: Building infrastructures to combine search & planning strategies with chemical data mining and modeling techniques; knowledge management, information integration (WEB 2.0), task-specific optimization of work flow and reporting in web-based chemistry; molecular (dis)similarity, structure-property (nanoarchitecture-property) relationships, virtual/combinatorial chemistry, screening and filtering, chemical safety and risk assessment, clean technology, nanoscience.

2011 **Founder** of the **CurlySMILES open-source project**, www.axeleratio.com/csm/proj/main.htm.

CurlySMILES integration in applications and interfaces is taking off:

- ***Molecular Material Informatics*** included CurlySMILES in their **Mobile Molecular Data Sheet** (**MMDS**) application as an exportable format for portable devices: molmatinf.com/mmdsios.html#section10;
- ***CGA Software Services*** applies CurlySMILES to encode **macromolecular structures**: ggasoftware.com/opensource/indigo/concepts;
- Materials Matter! reviewing portal, interfacing CurlySMILES-based queries for materials, including metal and semiconductor compounds, complexes, crystals and nanostructures, with brief factoids, which are backed by links to the original literature, commonly via the Document Object Identifier (DOI); the portal is interactive and accepts factoid and URL input by clients.

2001-2010 **Senior research affiliate** at Owens Technology, Inc., Palo Alto and Reno:

- Researched design and characteristics of sustainable and cost-efficient photovoltaic materials and devices by applying computer-aided methods to identify and optimize chemical precursors and reaction media in relation to semiconductor device properties and performance parameters;
- Developed the cheminformatics infrastructure for work & research flow (automatized management of the chemical inventory, material safety data and patent literature as well as the design and documentation of experimental protocols and clean room procedures);
- Coordinated cooperations with third-party laboratories to proceed with materials testing and characterization (spectroscopy);
- Investigated reactant/solvent systems and alternate systems based on room-temperature ionic liquids (RTILs) for electrochemical deposition of semiconductor layers and metal contacts as well as for surface modification of material interfaces;
- Integrated the open-access ThermoML archive for research needs by implementing data mining tools in combination with physicochemical estimation methods and predictive models.

1995-2000 **SFB-Project leader** and **teaching** at the Technical University of Freiberg (School of Mining), Germany:

- Installed 40 independent processor units for concurrent batch simulations under Linux;
- Developed random-walk models for amphiphiles and polymer molecules grafted on particle surfaces with varied nanostructured geometries to study interaction (dispersion, aggregation) of surface-modified particles and nanostructues;
- Implemented Monte Carlo simulation techniques in C++;
- Taught classes in physical chemistry and quantum chemistry and supervised student projects in scientific software development.

1989-1995 **Postdoctoral research affiliate** at the Terman Engineering Center, Stanford University, California:

- Developed and implemented models for property estimation, risk analysis and environmental fate and transport studies of organic compounds;
- Designed a new approach combining automatic molecular difference recognition and group contribution models to deduce properties of novel compounds from known data of structurally similar ones;
- Published a handbook on property estimation methods targeting high-risk chemicals, potential pollutants and intermediates;
- Participated in a cooperation with the company Aquateam in Norway and applied molecular modeling approaches to the design of testing and screening protocols for chemicals applied in off-shore oil drilling operations.

1988	Dissertation in Chemistry at the Institute of Organic Chemistry at the Technical University of Munich (Garching), Germany.
1984	Diploma in Chemistry at the Institute of Physical Chemistry at the *Georg-August* University in Göttingen, Germany.

Special Skills

Cheminformatics:	Design of mathematical formalisms to describe and analyze chemical systems; computer implementation of chemical tasks.
Molecular Modeling:	Molecular graph theory, molecular similarity, quantitative structure-activity relationships (QSARs), multivariate data analysis, scaling, *k*NN methods, hierarchical ordering and classification techniques, pattern recognition methods, scaling, Monte Carlo simulation.
Data mining:	Web 2.0, MySQL, ThermoML archive, Crystallography Open Database.
Programming:	Web applications, object-oriented programming (OOP), Python, Perl, PHP, Ruby, C++, JavaScript, HTLM5, CSS, XML; Mathematica, MAPLE.

Miscellaneous

Memberships:	American Chemical Society (ACS) and German Chemical Society (GDCh).
Science Fair:	ACS Judge for the awards of chemistry-related youth science projects competing at the Intel International Science and Engineering Fair in Reno, Nevada, in 2009.
Languages:	Fluent in English and German.
Eligibilities:	Eligible to work in the United States and the European Union.

Further Information and Publications

Further information will gladly be furnished upon request. Also, please find my profile and publications online: profiles.google.com/axeleratio/about; www.axeleratio.com/axel/articles.htm, ~/book.htm and ~/theses.htm.

References

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- Dr. Kristina Voigt, Institute for Biomathematics und Biometry, Ingolstädter Landstr. 1, 85764 Neuherberg, Germany, phone: ++49-89-3187 4029, e-mail: kvoigt@helmholtz-muenchen.de;
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