www.quantemolDB.com

QDB plasma chemistry

Validated Plasma Chemistries Database

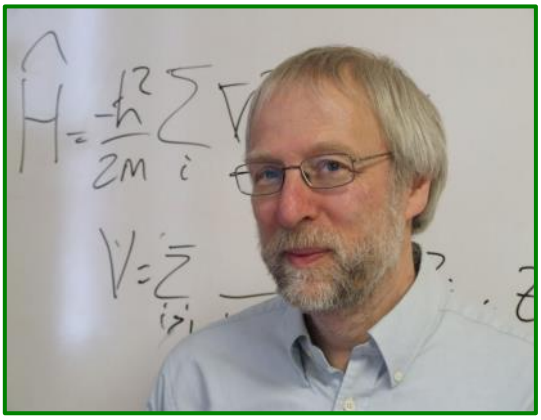
The QDB mission is to provide validated plasma chemistry data solutions to meet the ever changing demands of industrial and academic plasma modelling research

2019 Brochure

Quantemol

Company Profile

Quantemol was founded by Prof. Jonathan Tennyson FRS and Dr. Daniel Brown in 2004. The company develops unique software tools that bring accessibility to highly sophisticated research codes and unique data. Our projects include:



Quantemol-N uses the UK molecular R-matrix code to model electron-polyatomic molecule interactions.

Quantemol-VT brings an unsurpassed user experience to the world-renowned plasma simulation codes of Prof. Mark Kushner from the University of Michigan.

Quantemol-DB (QDB) is a leading sustainable database, representing the chemical and radiative transport properties of a very wide range of plasmas. The database contains chemistry data for plasma chemistry modelling with pre-assembled and validated chemistry sets, and is regularly updated with the most recent and relevant data.

With an expanding research team, Quantemol is able to offer **consultancy** projects that are carried out by world leading scientists in their respective fields.

Our mission statement is

"To serve our users in industry and academia, to simulate complex processes more efficiently, reliably, accurately and cost-effectively and thereby accelerate technological and scientific innovation".

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QDB plasma chemistry

Background

A better understanding of plasma chemistry has the potential to help address issues of global warming and pollution as well as enabling more technologies to be used to improve our standard of living and environment. Industries in which plasmas are frequently used include semiconductors, thin-layer manufacturing, plasma medicine, combustion, and agricultural applications of plasma to name a few.

The purpose of QDB is to provide a forum for collaborative efforts between academia and industrial research, allowing researchers to access, compare and improve their understanding of chemistry sets influencing plasma behaviour.

One of the most challenging aspects of plasma modelling is insufficient chemistry data. The lack of a unified and convenient database with complete and validated data sets impinges the ability to expand knowledge of plasma processes and widen their use in industrial applications.

Why Quantemol?

Quantemol is a market leader in providing unique cross-section data for plasma chemistry software and consultancy services in the field of plasma modelling.

Our advanced methods are employed to perform theoretical calculations and inform estimates for missing chemical reactions. Uncertainty quantification for simulations of the complex systems method is used to establish validation of the estimated data, where direct validation is not possible due to a lack of experimental data.

QDB contains chemistry data for plasma modelling with pre-assembled and validated chemistry sets.

QDB provides the world's largest, most accurate, validated, sustainable plasma chemistry data repository for its users

What is QDB?

The Quantemol chemistry database includes the following data and services:

- Complete chemistry sets for use in the semiconductor industry (mainly low pressure plasma conditions)
- Chemistry sets optimised for certain pressure regimes
- API and formats compatible with a range of software packages available (QVT, ChemKIN, COMSOL, CFD-ACE+, VisGlow etc)
- Automated chemistry generation using data in QDB and choice of feed stock gases
- Capacity for data comparison between individual reactions and assembled data sets
- Data download through a user-friendly interface
- Feedback on chemistry sets by users

Key advantages of QDB

- All data in one place: electron scattering, heavy particle collisions, surface chemistry – eliminating the need mix and match different sources
- Use the data with confidence. QDB uses only trustworthy and validated data that is monitored on a regular basis
- Save time on chemistry set search, comparison, and validation. Easy to use tools will help you to assemble the set you need in minutes
- Save time with QDBs intuitive interface for exporting data in flexible formats, avoiding human error
- Don't struggle alone - reach out to our active customer support
- Collaborate with us. Provide your feedback and request the data you want - we'll do our best to add it for you

Academic Advisory Board

Annemie Bogaerts

Professor of Chemistry, Research group PLASMANT University of Antwerp , Belgium.

Area of expertise: Plasma chemistry modelling, plasma reactor modelling, modelling plasma-surface interactions and experiments, mainly for environmental/energy and medical applications

Annarita Laricchiuta

Researcher, PLASMI Lab at CNR NANOTEC Bari , Italy

Area of expertise: state-resolved electron-molecule cross-section calculations, molecular structure.

Bastiaan J Braams

Physicist, "Centrum Wiskunde & Informatica (CWI)", the Dutch national centre for mathematics and computer science, the Netherlands.

Area of expertise: molecular modelling, potential energy surfaces, plasma physics, atomic and molecular data, molecular dynamics for scattering and spectroscopy

Christian Hill

Unit Head, Atomic and Molecular Data Unit, Nuclear Data Section,

International Atomic Energy Agency (IAEA), Vienna, Austria.

Area of expertise: database design, online interfaces, molecular spectroscopy, atomic and molecular data.

Christopher Whitehead

Emeritus Professor of Physical Chemistry, School of Chemistry, The University of Manchester, UK.

Area of expertise: Plasma chemistry. Use of atmospheric, non-thermal plasma for the removal and conversion of environmental pollutants and the production of high-value products and fuels from methane and carbon dioxide.

E. Krishnakumar

Senior Professor, Natural Sciences Faculty, Tata Institute of Fundamental Research, Mumbai.

Fellow, Indian Academy of Sciences, Bangalore.

Area of expertise: Measurement of electron ionization and dissociative attachment cross-sections, dynamics of molecular negative ions, photoionization and photodetachment, electron and ion spectrometry.

Jean-Paul Booth

Professor of Physics, CNRS Research Director at Laboratoire de Physique des Plasmas, Ecole Polytechnique, Palaiseau, France. Fellow of AVS.

Area of expertise: Laser and other optical diagnostics of plasmas in reactive gases. Physics and chemistry of radiofrequency plasmas for surface processing

Jonathan Tennyson

Massey Professor of Physics, Fellow of the Royal Society, Department of Physics and Astronomy, University College London, UK.

Area of expertise: electron molecule scattering cross-sections calculations, molecular structure and molecular spectroscopy

Academic Advisory Board

Julian Schulze

Associate Professor, Institute for Electrical Engineering, Ruhr-University Bochum, Germany. Research Professor, Department of Physics, West Virginia University, USA.

Area of expertise: Low temperature plasma science, plasma diagnostics and simulations.

Jung-Sik Yoon,

Deputy Director of Plasma Technology Research Center, National Fusion Research Institute, Korea.

Area of expertise: Atomic and molecular data evaluation, generation of plasma processing data set, and data analysis.

Khaled Hassouni

Professor of Physics, Director of Le Laboratoire des Sciences des Procédés et des Matériaux (LSPM), CNRS-INSIS, France.

Area of expertise: plasma diagnostics, low temperature plasma, analytical plasma modelling.

Klaus Bartschat

Levitt Professor of Physics, Fellow of the American Physical Society, Department of Physics & Astronomy, Drake University, Des Moines, Iowa, USA

Area of expertise: electron and photon collisions with atoms and ions.

Matthew Goekner

Fellow of the AVS

Professor of Physics and Associate Dean of Natural Sciences, University of Texas at Dallas Richardson TX,USA.

Areas of expertise: Experimental IR absorption and electron impact excitation cross-section measurements. Experimental and computational plasma physics.

Miles Turner

Professor of Physics, National Centre for Plasma Science Technology, Dublin City University, Dublin, Ireland.

Area of expertise: Plasma theory and simulation, plasma chemistry modelling, verification and validation.

Nigel Mason

Professor of Physics, Department of Physical Sciences, The Open University, UK .

Area of expertise: experimental electron molecule scattering cross-sections and molecular spectroscopy.

Satoshi Hamaguchi

Professor of Physics, Center for Atomic and Molecular Technologies, School/Graduate School of Engineering

Osaka University, Japan.

Area of expertise: theoretical and computational plasma physics, strongly coupled plasmas, plasma processing.

Academic Advisory Board

Uwe Czarnetzki

Professor of Physics, Ruhr-Universität Bochum, Institute for Plasma und Atomic Physics, Germany.

Area of expertise: Basic plasma physics, plasma sources, plasma diagnostics, spectroscopy, non-linear optics, atomic / molecular physics

Yi-Kang Pu

Professor of Physics Department of Engineering Physics, Tsinghua University, Beijing, China.

Area of expertise: diagnostics for low temperature plasmas, discharge physics, plasma instabilities, plasma source development.

Yuki Itikawa

Professor Emeritus, Institute of Space and Astronautical Science, Sagamihara, Japan.

Area of expertise: Theoretical studies of electron collisions with atoms and molecules and photoionization of atoms and molecules. Compilation and evaluation of atomic and molecular data.

Zoran Lj. Petrović

Professor of Physics, Fellow of the Serbian Academy of Sciences and Arts and of American Physical Society.

Institute of Physics, University of Belgrade, Serbia.

Area of expertise: electron molecule scattering, swarms and transport of electrons, positrons and ions, physics of ionized gases, gas discharges, plasma diagnostics and modeling, plasma applications including plasma medicine.

Industrial advisory board

Dr. Alok Ranjan

Manager & Senior Member of Technical Staff

TEL Technology Center, America, LLC, USA.

Area of expertise: Modeling & Simulation of Plasma Etch; Plasma Etch Process Development; Plasma Diagnostics.

Dr. Sumeet C. Pandey,

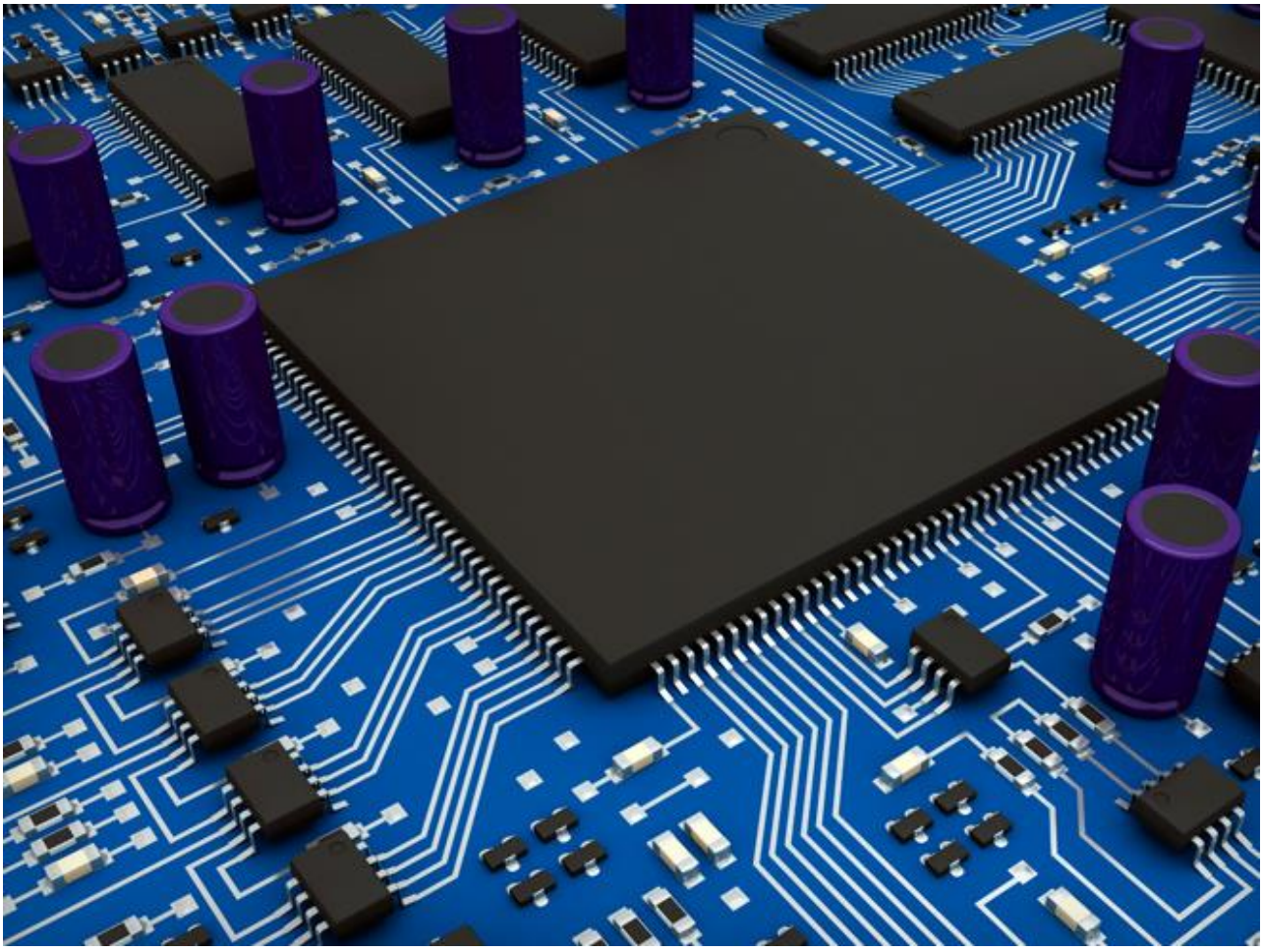
Principal Engineer, *ab initio* Research Lead, Technology Development, Micron Technology Inc.

Area of expertise: Atomistic simulations of plasma-material interactions for deposition and etch, First-principles-based materials and emerging device modelling, DFT-based calculations of surface and gas-phase chemistry and spectroscopy .

Dr. Shahid Rauf

Principal Member of Technical Staff and Senior Director
Applied Materials Inc., USA.

Area of expertise: Modelling of plasma processing systems, physics and chemistry of plasma materials processing.



Approach to validation

The principles established for the validation of chemistry sets are that:

1. There is experimental benchmarking from open sources (where available) and also directly provided by Quantemol's industrial partners (collaborating on the Powerbase project) and database contributors.

2. Calculations are performed for a range of models thereby reflecting the underlying quality of input data (example models used for validation include HPEM, Global_Kin, ChemKin).

3. The models used to produce the data are validated on a case by case basis.

4. Numerical uncertainties are quantified with thresholds set for validation where possible.

This methodology was specifically applied to atomic and molecular calculations using the principles established in the publication "Uncertainty Estimates of Theoretical Atomic and Molecular Data"[1], which was produced for the International Atomic Energy Agency and focused "on data that are most important for high temperature plasma modeling" with the "ultimate goal to develop guidelines for self-validation of computational theory for A+M processes".

It is recognised that while the validation of chemistry sets directly may still be uncertain, the validation of data produced by models using this data will often be more easily obtained.

QDB users are invited to validate and evaluate chemistry sets either directly or by validating the results of models which use these chemistry sets as inputs. Validation of the chemistry sets provided in the database will be based on the foundations of Uncertainty Quantification for calculations of complex systems [2,3].

Plasma researchers are encouraged to contribute to the validation process and receive 6 months free access to the subscription section of the database per contribution.

The chemistry set will be used for the modelling of different reactors. Comparison of the model output with measurement is the principal method for validation.

For chemistry simulation, the scaling law based on the parameter study is a common methodology for this validation [4]. For higher dimensional simulation, the behaviour of the species and the surface will be used for comparison [5].

Part of this chemistry will be validated by comparison of different measurements which are and will be available to us in the context of the Powerbase project and different academic research groups from the reviewer's panel.

We hope that the community will take part in the validation and subsequent scientific discussions, which will facilitate research in this field.

Comprehensive and complete referencing will be provided with users downloading chemistry sets, ensuring that relevant citations to chemistry set and validating experiments are included and can be used for publications.

References

1. http://www.siam.org/activity/uq
2. H. K. Chung et al "Uncertainty Estimates for Theoretical Atomic and Molecular Data", J. Phys. D 49 (2016) 363002.
3. National Research Council Committee on Mathematical Foundations of Verification, Validation and Uncertainty Quantification, Assessing the reliability of complex models: mathematical and statistical foundations of verification, validation and uncertainty quantification (National Academies Press, 2012)
4. Principles of Plasma Discharges and Materials Processing, Micheal A.Lieberman, Alan J. Lichtenberg, 1994,(John Wiley & Sons, 2005), ISBN 0-471-72001-1
5. Zhang, Da, and Mark J. Kushner. "Investigations of surface reactions during C2F6 plasma etching of SiO2 with equipment and feature scale models." Journal of Vacuum Science and Technology-Section A-Vacuum Surfaces and Films 19.2 (2001): 524-538.

Validation of Individual Chemistry Reactions:

Rate coefficients for each reaction are included in the validated chemistry set for a similar range of temperature and pressure.

The main validation method for individual reactions will be compared with alternative theoretical calculations/estimations and experimental measurements.

For unknown reactions different calculation methods include:

- Quantemol-N (R-matrix method) calculations for electron molecule scattering reactions
- Scaling law, mathematical methods of estimation and expert opinion to estimate necessary data
- Quantum and transition state theory for unknown heavy particle reactions

User data for validation is welcomed with 6 months free subscription; references to the contributors' original publications are included in publications using the data, and a bibliography provided with data downloads.

API feature

The *Application Programming Interface* (API) is a set of protocols and tools for linking the database with our plasma modelling software QVT. An API specifies how software components should interact and APIs are used when chemistries can be accessible in graphical user interface (GUI) of the plasma modelling software.

This will help users to save time and avoid human error when transferring the data to their models and keep chemistry data up to date, whilst the library of chemistry sets will be growing.

QDB is now featuring download format for COMSOL, ChemKIN, CFD-ACE+, HPEM, VisGlow plasma modelling software packages.

If you would like to use assembled chemistry sets including species, reactions and cross-section data in your plasma model you can easily download data in a compatiable format and proceed to modelling right away.

Surface Processes

Quantemol is developing a data model for representing surfaces and surface processes, and populating the database with relevant data. Surface reactions are validated as part of the chemistry set. The main parameters used for comparison are etching rate and deposition rate, where available.

Unknown surface reactions are estimated by scaling laws based on similar reactions.

Ideas on validation methods are very welcome.

Free of charge

Individual reactions in the form of cross rate coefficients are available for molecules, ionised, exited and vibrational states. The database has rigorous source referencing.

Subscribe to access a growing library of complete chemistry sets:

Ar	N_2/H_2	Ar/O_2	He/O_2
He	Ar/H_2	$Ar/O_2/C_4/F_8$	$CF_4/CHF_3/H_2/Cl_2/O_2/HBr$
H_2	O_2/H_2	$SiH_4/Ar/O_2$	CH_4/N_2
N_2	SF_6/O_2	Ar/Cu	$SF_6/CF_4/O_2$
O_2	CF_4/O_2	$Cl_2/O_2/Ar$	Ar/Cu/He
	SF_6	$Ar/BCl_3/Cl_2$	Ar/NF_3
	CF_4	Ar/NH_3	$SF_6/CF_4/N_2/H_2$
	C_4F_8	CH_4/H_2	$Ar/NF_3/O_2$
	SiH_4	C_2H_2/H_2	C_2F_6/SiO_2
	SiH_4/NH_3	CH_4/NH_3	CF_4 / SiO_2(s)
		C_2H_2/NH_3	$CF_4/O_2/N_2/H_2$ (1-30 mTorr)
		$CF_4/O_2/H_2/N_2$	O_2 (600 Torr)
			$BCl_3\backslash Cl_2\backslash Ar$ (1 - 10 mTorr)

Roadmap of Developments

Chemistry generator engine

The chemistry generator engine provides automatic generation of reactions, and suggests a complete set of gas phase and surface reactions tailored to a particular pressure range. Automatically generated reactions are based on gas mixtures and species in the plasma as defined by the user during the input stage. The model generates a full list of species which may be present in the plasma but which have different probabilities of existence. The set of species can then be modified and any unphysical species removed.

The full variety of the species is listed — allowing users to decide which species could be removed from the plasma chemistry being designed.

Next, the database of reactions is scanned for those containing generated chemistry species. Species which only presents only on one side of the equation are highlighted so that the user can see potentially important missing pathways.

Important missing reactions can be estimated or calculated by different approaches by Quantemol consultants so providing a complete tchemistry set.

ChemGen v 1.0—Beta version

The initial version of Chemistry generator helps to gather data which is already in QDB related to feedstock gases of the plasma.

User has flexibility to choose which species and which reactions they want to download and the format they want to download in. Download is only available for Gold members.

Try it now

www.quantemolDB.com/chemistries/dynamic-chemistry

Price List*

Membership	Product	Annually*	3 years*
Basic	Access to individual chemical reactions from public domain	FREE	FREE
Academic	Additional access to pre assembled most common chemistry sets to be used in non commercial research	£2,000	£4,500
Industrial	Additional access to pre assembled most common chemistry sets be used in	£5,280	£13,200
	Individual reaction calculation request	PPA	
	Individual chemistry design and validation request	PPA	

* - all prices are quoted excluding VAT

Additional IDs - additional users in the same organisation are charged at 10% of the membership price.

Commercial research - research by commercial organisations or for commercial organisations where results that are not made publicly available

Non-commercial research - research by not-for-profit organisations producing publishable results

Quantemol Database Terms policy

The details on general terms of use and privacy policy can be found here: www.QuantemolDB.com/about/legal/

Become A Gold Member And Receive More Benefits

- Access to pre-assembled and validated chemistry sets
- Functionality to download cross-sections and chemistry sets in flexible text format
- Customer support helping to tailor our chemistry sets to user's plasma model
- Help in assembling user's own chemistry set
- Ability to leave feedback on data and read feedback from other users
- Free participation in plasma chemistry design workshops and webinars
- Access to API for QVT and download data formats tailored for popular plasma modelling software
- Access to Chemistry Generator downloads (5 chemistries downloads/ month)
- Up to 6 chemistries/1000 reactions can be downloaded a month (monthly renewal)

CONSULTANCY

As well as providing advanced modelling software, Quantemol provides a unique consultancy service. With our suite of software and highly skilled engineers, we provide extensive and in depth analysis tailored to specific customer requirements. Consultancy projects range from small quick calculations work to comprehensive plasma chemistry development. Typical types of consultancy work provided are:

- Calculation of specific electron-molecule cross-sections including:
  - ⇒ Electron impact dissociation cross-sections producing specific products
  - ⇒ Electron impact ionisation dissociation producing specific products
- Heavy particle collision cross-section calculations for neutral particles colliding
- Vibrational excitation cross-section calculation for diatomic molecules and ions
- Industrial plasma tool simulations
- Plasma process parameter optimisations
- Plasma chemistry designs
- Plasma etching and deposition calculations
- General multiphysics problems (CFD, etc..)

Quantemol has successfully undertaken several large consulting projects. A distinctive feature of our service is that we work with non-standard requests, using computational methods and literature research in order to achieve the results within deadlines. We always strive to deliver results of value to our customers and prioritise research tasks according to our client's development needs. A formal completion report is produced at the end of all work providing the results (raw data, graphs, videos etc..) ready for use and presentation. We work on the basis of complete confidentiality and understand the importance of protecting intellectual property.