www.quantemolDB.com

QDB plasma chemistry

Validated Plasma Chemistries Database

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

2020 Brochure

Quantemol

Company Profile

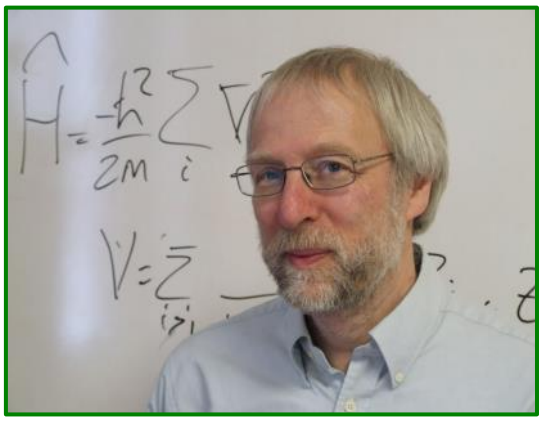
Quantemol was founded by Prof. Jonathan Tennyson FRS and Dr. Daniel Brown in 2004. The company develops unique software tools that bring accessibility to highly sophisticated research codes and unique data. Our projects include:

Quantemol-N Quantemol-EC use 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 carried out by world-leading scientists in their respective fields.



Prof. Jonathan Tennyson, FRS, UCL

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."

Contact Details

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QDB plasma chemistry

Background

Plasma chemistry has the potential to help address some of the world's most complex issues such as global warming and pollution. It has already enabled technologies which improve our standard of living and environment. Semiconductors, thin-layer manufacturing, plasma medicine, combustion and agriculture are just some of the industries in which plasmas are frequently used.

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. Access to a unified and convenient database with complete and validated data sets allows businesses to expand their 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.

QDB contains chemistry data for plasma modelling with pre-assembled and validated chemistry sets, applications allowing users to assemble their own sets and run Global model and Boltzmann Solver online.

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:

- Database search for reactions and species
- Flexible graphs for cross sections data
- Over 40 pre-assembled chemistry sets
- Dynamic Chemistry Generator app to make the reactions list for a new chemistry
- Download up to 20 datasets/month for FREE
- NEW! Boltzmann solver online
- NEW! Global Plasma Model available online
- Request a chemistry set optimisation

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 QDB's 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.

QDB beyond just data

QDB includes various types of data which is of interest for plasma modellers.

Data Model:

Species

- Reactions (cross sections/rates)
- Electron, heavy particle, photon
- Thermodynamic (soon)
- Full bibliographic records
- Pre-assembled (and validated) chemistries

QDB includes not only a comprehensive library of reactions data but additional functionalities enabling members to use the data and address their questions about plasmas.

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.

Surface Processes

Quantemol is developing a data model for representing surfaces and surface processes, and populating the database with relevant data.

QDB now also hosts some data for surface processes split into two categories: Data for plasma simulations such as sticking coefficients and data for surface models (site-base or feature profile).

We currently have sticking coefficients for atomic oxygen, atomic fluorine, fluorocarbons, and silane radicals.

For surface mechanisms such as specific etches, the database provides a set of individual reactions with their associated probabilities.

For energy-dependent reactions, the formula and the value of the used parameters is given.

These sets can be used in site-based or feature profile models.


Etching Mechanisms: Chemical Silicon Etch with Fluorine II

Based on sticking coefficients calculated via molecular dynamics

The values for individual coefficients depend heavily on the exact surface composition. They should be interpreted as guidelines rather than exact values.

Reaction	Formula	Coefficients	Comment
F + Si(s) -> SiF(s)	-	0.98	Between 173 K and 300 K
F + SiF(s) -> SiF_2(s)	-	0.93	Between 173 K and 300 K
F + SiF_2(s) -> SiF_3(s)	-	0.60	Between 173 K and 300 K
F + SiF_3(s) -> SiF_4 + Si(s)	-	0.24	Between 173 K and 300 K

S. Tinck, E. C. Neyts, A. Bogaerts, "Fluorine–Silicon Surface Reactions during Cryogenic and Near Room Temperature Etching", *J. Phys. Chem. C* **118**, 30315 (2014). [link to article] [B600]

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)

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 compatible format and proceed to modelling right away.

Data applications

RECTION SELECTIONAND DOWNLOAD	BOLTZMANN SOLVER	GLOBAL MODEL

FEED GASES

- ☐ Al
- ☐ BCl_3
- ☐ C_4F_6
- ☐ Ar
- ☐ C_2H_2
- ☐ C_4F_8

Dynamic Chemistry app

This is application helps to gather data which is already in QDB related to feedstock gases of the plasma and assemble your won set quickly.

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 and Platinum members.

Global Model app

After picking the chemistry set users have an option to run a Global Model right there on QDB. It reads QDB data in Arrhenius form fitted to cross-sectional kinetic data. The global model calculates the reactor averaged particle densities and the electron temperature for a given set of process parameters.

Currently the online model assumes constant power, however shortly it will be upgraded to include pulsing.

Solving equations:

* Particle density balance for heavy species
* Charge neutrality
* Electron energy density balance

The model is a simplified tool to give you some idea about the scale of the species concentrations and dominant species.

A detailed documentation can be found here.

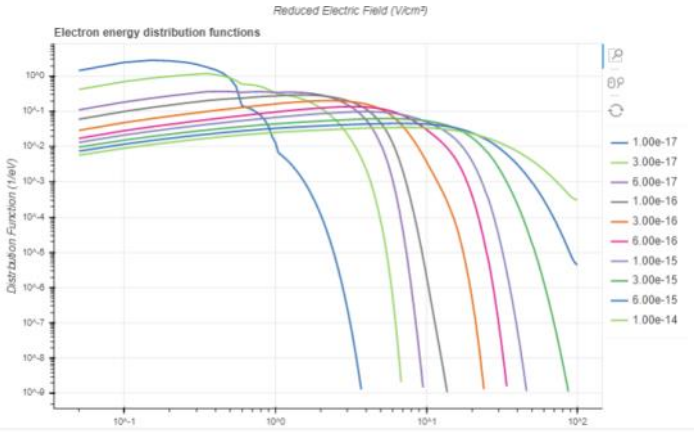
We have access to more advanced Global Models in-house and can offer consultancy services calculating surface chemistry interactions and other properties.

Boltzmann Solver

If you are working with non-Maxwellian distributions and need to obtain suitable reaction rates quickly there is another handy tool on QDB: Boltzmann Solver. It is based on the formalism described in S. D. Rockwood, "Elastic and Inelastic Cross Sections for Electron-Hg Scattering from Hg Transport Data", *Physical Review A* **8** , 2348-2358 (1973). It was extended to a non-uniform energy grid.

Calculations can be set up for both pre-assembled and self-generated chemistry sets. Only inputs are the relative densities of relevant species and the neutral gas temperature.

As a default, the feed gases are taken into account. For reactive gases or suspected high densities of excited/charged species, additional species from the chemistry set can be added by the user.



The solver calculates EEDFs, effective electron temperature, and rate coefficients for electron collisions in the chemistry set you selected for a gas temperature of choice.

Industrial advisory board

Dr. Alok Ranjan

Manager & Senior Member of Technical Staff

TEL Technology Center, America, LLC, USA.

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

Dr Ankur Agarwal

Director at KLA Corporation, USA.

Area of expertise: Hardware design, manufacturing process development and modelling of plasma processes for various stages of microelectronics device fabrication.

Dr Saravanapriyan Sriraman

Technical Director,

Lam Research Corporation, USA.

Area of expertise: Product development and engineering, multi-scale modelling and simulation of plasma processing and plasma-material interactions; physics and chemistry of plasma materials processing; plasma diagnostics; plasma etch process development.

Dr. Shahid Rauf

Principal Member of Technical Staff and Senior Director

Applied Materials Inc., USA.

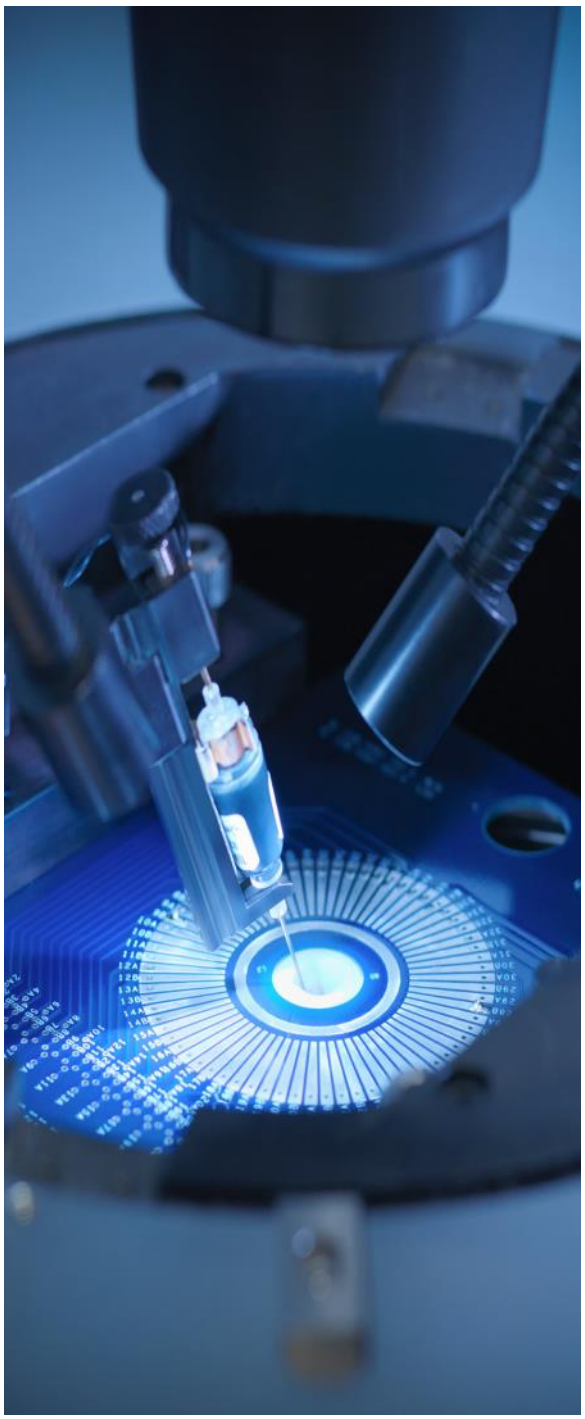
Area of expertise: Modelling of plasma processing systems, physics and chemistry of plasma materials processing.

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 .



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.

Luis Lemos Alves

Professor of Physics, Instituto Superior Técnico, Universidade de Lisboa, Portugal
Head of group N-Plasmas Reactive: Modelling and Engineering (N-PRiME) with Instituto de Plasmas e Fusão Nuclear.

Area of expertise: Plasma modelling and simulation, fluid modelling of dc/rf/microwave reactors, kinetic modelling using Chemistry-Boltzmann solvers, data assessment, verification and validation

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.

Academic Advisory Board

Peter Bruggeman

Professor of Mechanical Engineering and Associate Department Head, University of Minnesota, Minneapolis, MN, USA

Director High Temperature and Plasma Laboratory

Area of expertise: Plasma diagnostics, non-equilibrium plasma physics and chemistry, plasma technologies for environmental, chemical, energy, biomedical and decontamination application, plasma-surface interactions, multiphase plasmas in and in contact with liquids.

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.

Tatyana Rakhimova

Leading scientist, Head of theoretical Group, Microelectronics Department, Skobeltsyn Institute of Nuclear Physics at Moscow State University, Russia

Area of expertise: Physical processes in gas discharges, plasma chemistry and plasma-surface interaction.

Timo Gans

Professor of Low Temperature Plasmas, Head of Research in the Department of Physics, University of York, UK

Areas of expertise: plasma science and technology, advanced optical diagnostics, computational modelling, plasma dynamics, chemical kinetics.

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.

Price List*

Membership	User	Annually*	3 years*
Standard	Academic/ Industrial	FREE	FREE
Gold	Academic	£2,000	£4,500
Gold	Industrial	£5,280	£13,200
Platinum	Academic	£5,000	N/A
Platinum	Industrial	£15,000	N/A

* - all prices are quoted excluding VAT

Additional IDs - additional users in the same organisation will be offered a discounted price.

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

Academic research - research by not-for-profit organisations producing publishable results

Standard

- Database search for reactions and species
- Flexible graphs for cross sections data
- Use Dynamic Chemistry Generator app to make the reactions list for a new chemistry
- NEW! Download up to 20 datasets/month

Gold

- Database search for reactions and species
- Access to over 40 pre-assembled chemistry sets
- Use Dynamic Chemistry Generator app to make the reactions list for a new chemistry and download it in a flexible format
- NEW! Download UNLIMITED datasets/month
- NEW! Download up to 20 Chemistry sets/month
- NEW! Download up to 20 Dynamic Chemistry sets/ month
- Flexible graphs for cross sections data
- Download data in flexible software formats: COMSOL, Chemkin, VIsglow, CFD ACE +, QVT
- Customer support on working with chemistry data

Platinum

- All benefits of the Gold membership
- Calculations of cross sections* for up to 6 molecules/ions within the membership 1-year term.
- Cross sections included* in the deal are here:
  - Electronic excitation cross-sections
  - Quenching cross-sections
  - Electron impact dissociation
  - Estimate dissociative electron attachment
  - Electron impact ionisation at all energies
  - Estimate branching ratio for electron impact ionisation and dissociation
  - Vibrational cross sections for diatomic molecules (N2, FO, CF etc)
  - and more…
- A comprehensive report about the calculations and data in any format you require

* - Calculations choice will be at the discretion of Quantemol, i.e. if there are specific cases where no reasonable calculations are possible the member will be informed and justification provided. We will make our best efforts to deliver for all of the requests.

Quantemol Database Terms policy

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

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.