QDB: Validated Plasma Chemistries Database

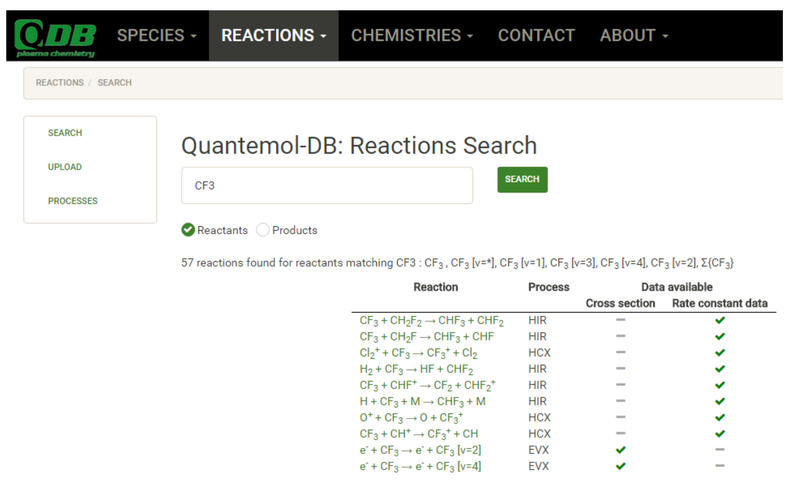
Sara Rahimi[1], James Hamilton[1], Christian Hill[1], Jonathan Tennyson[2]
1. Quantemol Ltd., London, NW3 4HA, UK
2. Physics & Astronomy, University College London, London, WC1E 6BT, UK

Quantemol Ltd
Quantemol is based at University College London and 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

QDB plasma chemistry

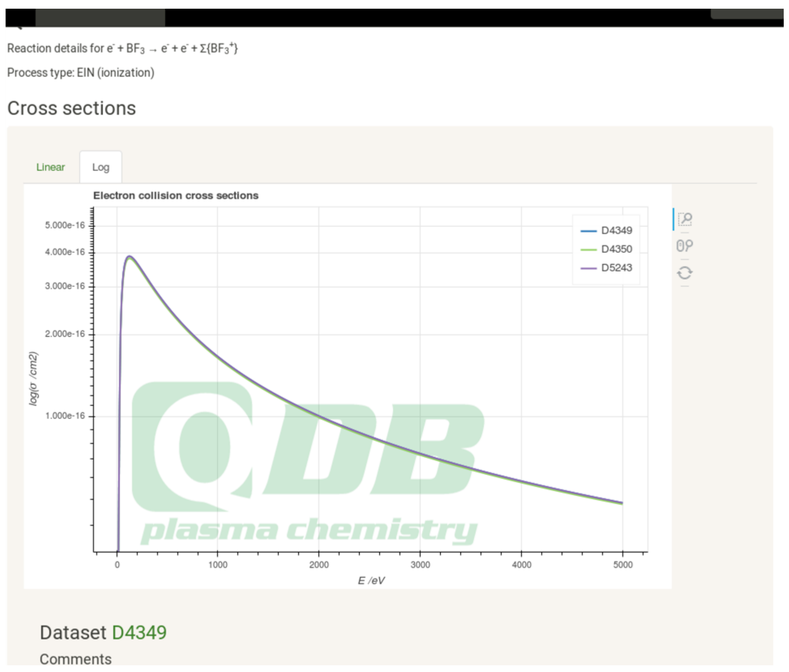
- Developed for people working on plasma modelling with complex chemistries.
- Supports and compares multiple data sets.
- Quantemol has developed a plasma chemistry database to establish a trusted resource for plasma chemistry information.
- Chemistry sets will soon be available for different plasma modelling software packages via API

Quantemol database provides:
- On going data updates and support
- Self-consistent and validated chemistry sets
- One place to exchange data and research ideas



Data Model

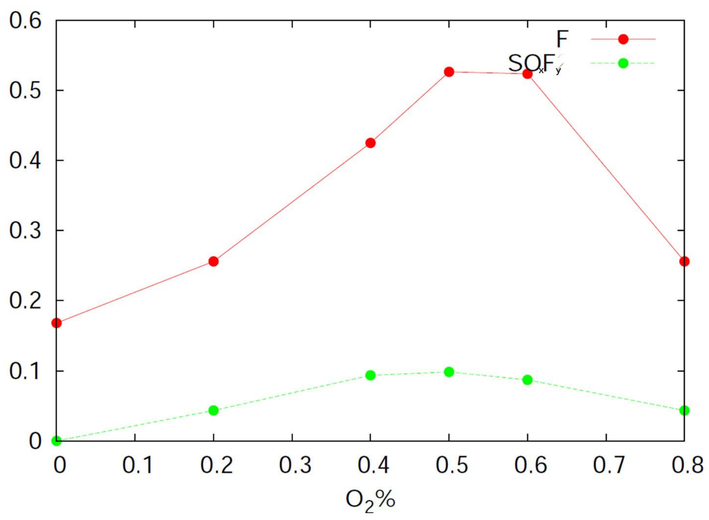
In QDB reactions and chemistries are presented in linked tables in a relational database. This allows users to make searches of the database to retrieve cross section and Arrhenius parameter data with visualization in their browsers.
Pre-assembled chemistry sets can be downloaded in one file in a flexible format.



Data sets: 5054 Cross sections: 2863
Reaction rates: 2189 Species: 931 in different states
Chemistry sets: 25

Validation via comparison to other sources: SF_6/O_2

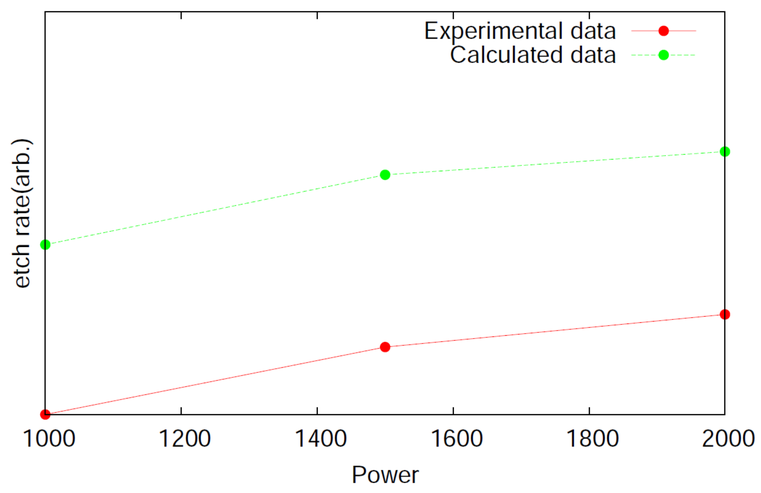
The validation was performed by comparing the simulation results based on an SF_6/O_2 chemistry created from reactions of the Quantemol database (QDB) with findings from [1]



Calculated percentage of molar productions for F and SO_xF_y in SF_6/O_2 plasmas as functions of mole percent of O_2. The total flow rate is 400 sccm at a pressure of 100 mTorr. Similar trends were calculated in [1].

Validation via using experimental data from an industrial partner: $SF_6/O_2/CF_4$

The Validation for $SF_6/O_2/CF_4$ was done by comparing the simulation with experimental results produced by Infineon AG for a back-side silicon etch.



The figure shows the etch rate of Si in an $SF_6/O_2/CF_4$ discharge at a pressure of 400 mbar. The goal of the modelling is to identify the optimum macroscopic plasma process parameters which give both a radially uniform etch and a short processing time (i.e. increase in yield).

References
1.Ryan, K. R., & Plumb, I. C. (1990). A model for the etching of silicon in SF6/O2 plasmas. *Plasma Chemistry and Plasma Processing*, 10(2), 207-229.

This project has received funding from the Electronic Component Systems for European Leadership Joint Undertaking under grant agreement No 662133. This Joint Undertaking receives support from the European Union's Horizon 2020 research and innovation programme and Austria, Belgium, Germany, Italy, Netherlands, Norway, Slovakia, Spain, United Kingdom