Quantemol database

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Need for plasma modelling

Plasmas for Energy and Environmental Applications ranges from environmental hazard mitigation to the use of plasmas to process agricultural by-products to water purification.

Crucial role of plasma modelling:
• help better understanding
• bring out new potential applications.

Examples:
• Pulsed discharges can aid low-cost processing of T-sensitive materials & treatment of contaminated water. Modelling is challenging: need for a comprehensive plasma chemistry set
• Plasma chemistry models for energy conversion and fuel and chemical synthesis (CO$_2$ to chemicals/energy). Complete chemistry sets need to include vibrational excitation cress section data for CO$_2$

Plasma chemistry for modelling
eg Argon
Quantemol has developed a plasma chemistry database to provide a trusted source of plasma chemistry information.

- For scientists working on plasma modelling with complex chemistries.
- Supports and compares multiple data sets.
- Chemistry sets can be used in different plasma modelling software via API.

**Quantemol database provides:**
- Ongoing data updates and support
- Self-consistent and validated chemistry sets
- One place to exchange data and research ideas
Advisory board team

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Self-consistent and validated chemistries

Chemistry network for SF₆/CF₄/O₂
Current numbers

Data sets: 4441
Cross sections: 2430
Reaction rates: 2111
Species: 841 in different states
Chemistry sets: 25

+ increasing
Data quality

Comparison with trustworthy open source data such as:

- Itikawa
- Christophoroou
- Zatsarinny + Bartschat
- Phelps
- Janev
- Quantemol’s own published data
Compare data

- Capacity to compare data sets for reactions and chemistry sets makes analysing data easier
- Data sheets for chemistry sets where users provide feedback
Validation

1. Experimental benchmarks
   • from open sources (where available)
   • provided directly by Quantemol’s industrial partners (e.g., H2020 Powerbase project)
   • database contributors.

2. Calculations performed for range of models reflect underlying quality of input data: models include HPEM, Global_Kin, ChemKin.

3. Validation of individual data sets: performed on a case-by-case basis.

4. Numerical uncertainties will be quantified and thresholds set for validation where possible.

Future development plan

End of 2016: API interface feature: access chemistry sets from within your plasma modeling software

Early 2017: Chemistry generator engine using mathematical models to generate possible species and discard unphysical ones in order to scan the database for reactions with physical species and provide user with tips and estimations for self-consistent chemistry construction.

Your suggestions are welcome!
Join Q-DB to benefit from:

- Trustworthy and validated data for plasma modelling
- Time saved on chemistry set search, comparison and validation
- Easy to use interface importing and exporting data in flexible formats
- Active customer support
- Help with referencing publications
- Compatibility with the most commonly used plasma modelling software
- Provision of the set based on customer demand.
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Thank you for your attention!

Database goes live
1 September 2016:
www.quantemolDB.com