

Quantemol-DB: A species and reaction database for plasma applications

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The importance of computer simulations for the understanding of plasmas and the design of reactions is ever growing. However, accurate results can only be obtained with detailed knowledge about the chemical reactions both between electrons and heavy particles and between different heavy particles. This information is often scattered over several publications, so assembling a chemistry set for a given problem is an arduous task. To assist with a fast assembly of reaction sets from reliable sources, Quantemol started the Quantemol-DB project, an online database of species and reactions related to plasma applications.

The Quantemol-DB comprises a large collection of species and reactions along with either cross sections or reaction rate coefficients. It is currently primarily aimed at low temperature plasma applications but can easily be extended to other fields such as fusion plasmas. The database is complemented by some additional functionalities such as pre-assembled chemistry sets and a tool to assemble custom chemistry sets from the database. The assembled data can be downloaded in formats compatible with common simulation programmes such as COMSOL.

This presentation will give an overview over the underlying data model, with an emphasis on the classification of excited species and reactions, and a demonstration of the website interface.