

Quantemol Plasma Chemistry Generator

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Quantemol Ltd was founded by Prof. Jonathan Tennyson and Dr Dan Brown in 2004 to develop unique software tools which bring accessibility to highly sophisticated research codes in the area of plasma physics. The Quantemol Database contains data on over 17000 electron and heavy-particle collision reactions. These are manually assembled into chemistries which are important when modelling industrial plasma etching and deposition processes. We present a new tool automating the process of assembling reactions into chemistries appropriate to the user's needs, and extending chemistries beyond the reaction data available in plasma chemistry databases. This forms the basis for a machine-learning approach to constructing valid chemistries and generating new data for reactions on which there is little computational or experimental information available.