

Real World Electron Cross-Section Calculations: *How Quantemol's QEC Software Accelerates R&D*

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Plasma physics and molecular modelling sit at the centre of many modern industrial processes, from manufacturing the nanoscale components inside smartphones to securing the high-voltage electrical grids that distribute power. The fundamental catalyst behind these technologies is the physical interaction between electrons and molecules. However, engineers and physicists face a major hurdle in advancing these fields: there is a lack of data regarding exactly how electrons collide with complex, rare, or highly reactive molecules. Gathering this cross-section data experimentally is frequently too expensive, technically demanding, or entirely impossible for transient species that exist for only fractions of a second.

QEC software provides a direct computational solution to this bottleneck. By packaging the highly sophisticated UKRmol+ R-matrix engine into an accessible graphical user interface, QEC allows researchers to calculate high-precision scattering data without needing to be an expert in command-line programming. This allows both specialists and non-specialists to run complex quantum chemistry simulations and overcome experimental limitations.

This document reviews three scientific studies where research teams successfully used QEC to resolve critical data scarcities and advance industrial and fundamental research.

Application 1: Securing the Electrical Grid with Sustainable Gases

Reviewed Study: Flynn et al. (2023), *Journal of Physics D: Applied Physics*

The electrical power industry relies on insulating gases to prevent catastrophic electrical sparks and arcs inside high-voltage switchgear and switchboards. Historically, sulphur hexafluoride (SF_6) was the industry standard, but it is an exceptionally potent greenhouse gas. Replacing SF_6 requires alternative insulating gases, such as the lower carbon alternative, fluorinated nitrile $\text{C}_4\text{F}_7\text{N}$. Developing accurate kinetic models to evaluate the safety and electrical strength of $\text{C}_4\text{F}_7\text{N}$ was previously hindered by the difficulty and expense of experimentally measuring its collision cross-sections.

In this study, Flynn et al. utilised QEC to calculate a complete and consistent set of electron-neutral collision cross-sections for this complex feed gas. QEC enabled the research team to compute elastic momentum transfer, electronic and vibrational excitation, and dissociative electron attachment cross-sections across a wide range of electron kinetic energies. These advanced calculations were executed through static exchange with polarisation (SEP) and close-coupling (CC) methodologies within the QEC suite. The resulting cross-sections were subsequently used in kinetic models to accurately calculate macroscopic rate and transport coefficients, bulk electron mobility, and critical electric field strengths. This work established the viability of $\text{C}_4\text{F}_7\text{N}$ as a sustainable high-voltage insulator, providing the foundational dataset needed for future eco-friendly power grid designs.

Application 2: Engineering Next-Generation Microchips

Reviewed Study: Bang et al. (2025), *ACS Applied Nano Materials*

The constant push for smaller microchips relies on advanced semiconductor lithography techniques, such as Extreme Ultraviolet (EUV) and Blue-X lithography. These methods use extremely short wavelength light sources to generate secondary electrons, which then interact with light-sensitive materials known as photoresists to induce chemical transformations and etch nanoscale circuit patterns onto silicon wafers. To engineer thinner, more resilient photoresists capable of sub-11 nanometre resolution, Bang et al. investigated a new inorganic molecular resist called TH-TMCTS. Understanding how this resist cross-links under electron exposure required precise atomic and molecular data regarding electron-induced reactions.

To uncover the exact reaction mechanisms, the researchers used QEC to calculate the excitation cross-sections of the molecule. This data enabled the neutral dissociation cross sections for the primary molecular bonds to be found, revealing that the dissociation cross-sections for Si-OH, SiO-H, Si-CH₃, SiCH₂-H, and core Si-O bonds are remarkably similar in magnitude. This generated the vital physical insights needed to confirm that all primary bonds can undergo dissociation concurrently under electron impact. As a result, the authors gained a comprehensive understanding of the resist's chemical contrast mechanism and confirmed its exceptional dry-etch resistance, paving the way for finer, more reliable semiconductor manufacturing.

Application 3: Cleaner Engine Technologies via Plasma Combustion

Reviewed Study: Ding & Liu (2025), *Physics of Fluids*

Plasma-assisted combustion is an innovative technology that introduces low-temperature plasma into a fuel mixture to enhance flame stability, increase combustion speed, and significantly reduce pollutant emissions. To accurately model and optimise plasma-assisted combustion systems, scientists require exact collision data for both primary fuel molecules and the short-lived, highly reactive free radicals created during plasma discharge. For ethane (C₂H₆), a primary component of natural gas, collision data for its first free radical, the ethyl radical (C₂H₅), is virtually non-existent in scientific literature because radicals react too quickly to be easily measured experimentally.

Ding & Liu applied QEC to perform calculations for low-energy electron scattering with both C₂H₆ and the transient C₂H₅ radical in the energy range of 0.1 to 15 eV. The authors calculated elastic scattering, momentum transfer, electronic excitation, and ionisation cross-sections for both species, alongside vibrational excitation cross-sections for C₂H₆. Beyond the scope of this paper, the new QEC 3.0 release will also enable the calculation of vibrational excitation for radicals such as C₂H₅.

The calculated elastic scattering, momentum transfer, and ionisation cross-sections for C_2H_6 demonstrated excellent agreement with existing experimental and theoretical benchmarks. By providing the missing cross-section set for the reactive C_2H_5 radical, the study delivered a dependable kinetic dataset to characterise plasma flow dynamics and reaction mechanisms in low-temperature combustion models.

Strategic Advantages of QEC and Improved Functionality

The strategic value of QEC lies in its ability to translate highly complex quantum physics into a user-friendly format, eliminating the bottlenecks traditionally associated with theoretical chemistry. The table below outlines how QEC's core features directly translate into practical research advantages, and highlights some key improvements in the most recent QEC 3.0 update:

Capability	Practical Benefit
Accessible R-Matrix Computing	The intuitive graphical user interface removes the steep learning curve associated with manual script configuration for the underlying UKRmol+ code engine, opening computational physics to wider scientific and industrial use.
Integrated Open-Source Quantum Chemistry Software	The newest release of QEC bundles PySCF directly into the platform for molecular geometry optimisation and orbital data, providing a ready-to-use alternative alongside the existing option for paid Molpro support.
Comprehensive Data Outputs	Generates comprehensive sets of exportable elastic and inelastic scattering data. Version 3.0 introduces an integrated Molecular Loader that simplifies job setup by minimising external inputs, while expanded cross-section data provision now supports radicals with vibrational excitation capabilities.
Accelerated Research Cycles	Replaces complex theoretical setup or costly experimental beam measurements with automated, parallelised computations that deliver results fast.

Ready to Advance Your Plasma and Materials Research?

Whether you are investigating sustainable insulating gases, engineering nanoscale photoresists, or modelling low-temperature combustion kinetics, QEC provides the computational foundation to resolve your data scarcity. Stop relying on incomplete datasets or spending months configuring manual calculations.

Evaluate how QEC can accelerate your research and deliver high-precision cross-section data for your specific molecular applications. Plus, the latest release of QEC (version 3.0) brings powerful new features and system upgrades. Read about the new features on our [blog](#).

- **Request a Free Trial:** Test the QEC interface and run your own calculations at quantemol.com/free-trial.
- **Consult Our Experts:** Discuss your precise modelling requirements with our team via sales@quantemol.com

References

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