Collision Ahead – An Electron Collision Cross Section Set for Water Molecules for Use in a Two-Term Boltzmann Solver

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Introduction

Water is an omnipresent impurity in vacuum applications [1]. H_2O molecules do not only interfere with the heavy particles but also with the free electrons, e.g. in plasma applications. A common description of the electron kinetics is the solution of the electron Boltzmann equation in the two-term approximation, e.g. by LoKI-B developed at IST Lisbon, yielding the electron energy distribution function (EEDF). However, for water no complete and consistent set of electron collision cross sections (CS) is openly available. For that reason, a set is proposed that includes, but is not limited to, a rigorous treatment of rotational collisions by means of the Born approximation and considers the anisotropy of the scattering process starting from the differential CS [2, 3]:

$$\left.\frac{\mathrm{d}\sigma(\varepsilon,\theta)}{\mathrm{d}\Omega}\right|_i = \sqrt{\frac{\varepsilon'}{\varepsilon}}\frac{4D^2}{6(2J'+1)}\frac{S_i}{\varepsilon'+\varepsilon-2\sqrt{\varepsilon'\varepsilon}\cos\theta},$$

to calculate individual integral and momentum transfer CS. For immediate applicability in any Boltzmann solver, an effective CS set is proposed as well.

Cross Section Set

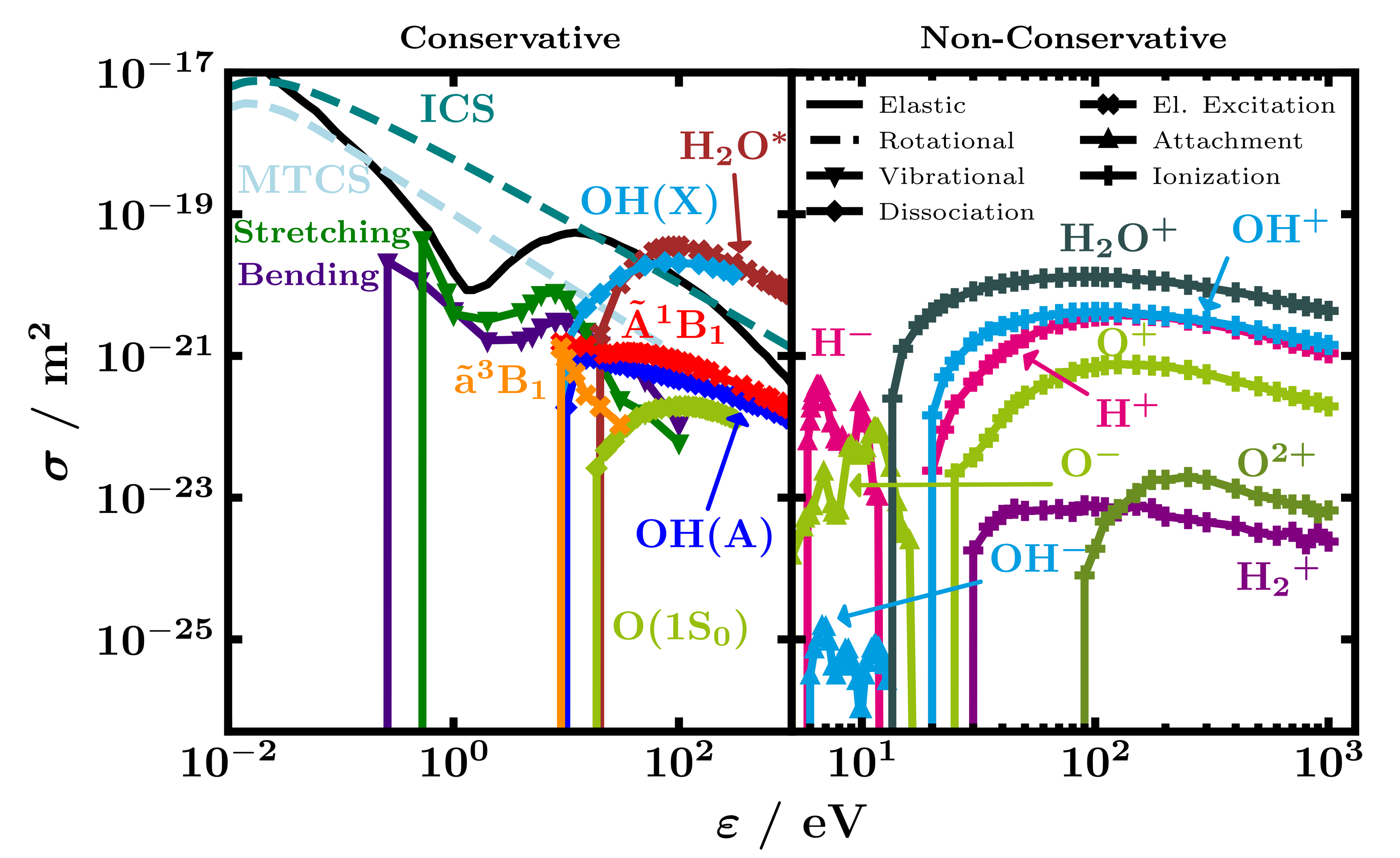

Fig. 1: Proposed complete and consistent electron collision cross section set for water molecules divided in conservative (number of electrons is constant) and non-conservative (ionisation and attachment) collisions.

Applicability

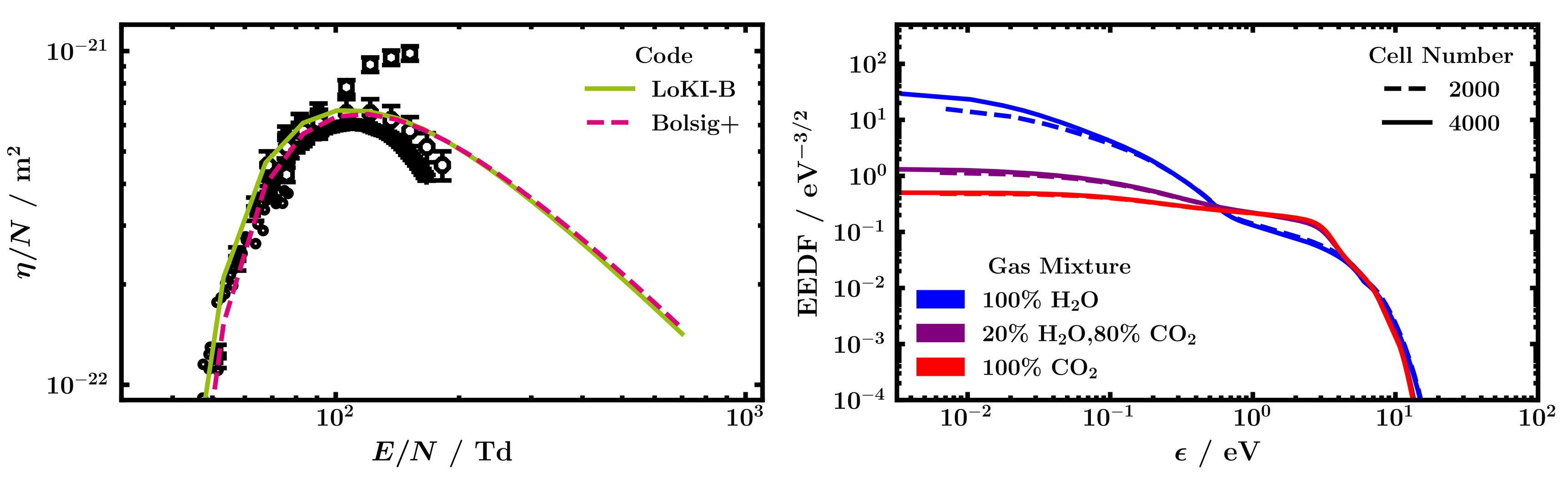

Fig. 3: Agreement of LoKI-B results with Bolsig+ (left), EEDFs for different gas mixtures with the proposed CS set at 70 Td (right).

Conclusion

- Rigorous description of rotational collisions of H_2O requires anisotropy
- Proposition of complete and consistent set of electron collision cross sections for use in anisotropic LoKI-B
- Immediate applicability in any Boltzmann solver due to additionally proposed effective CS set
- Both sets will be made available in the IST database with LXCat [4]

Validation

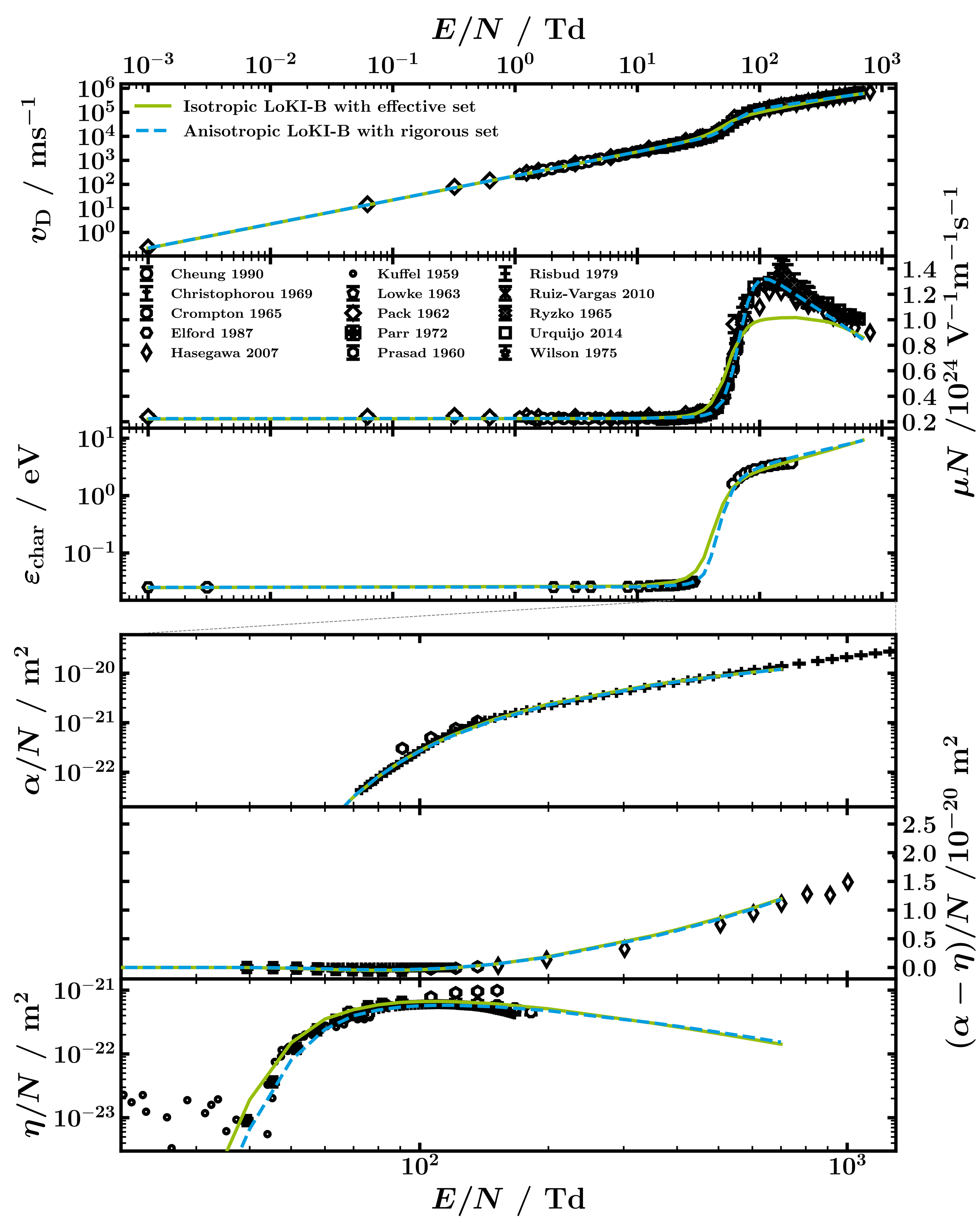

Fig. 2: Comparison of experimental electron swarm parameters - from top to bottom: drift velocity, red. mobility, char. energy, red. Townsend coef., red. eff. Townsend coef. and red. attachment coef. - with LoKI-B results using either the rigorous set in fig. 1 or a slightly adapted effective set.

Literature

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