Electron collision cross sections for H_2 and NH_3 relevant to N_2-H_2 plasma modelling

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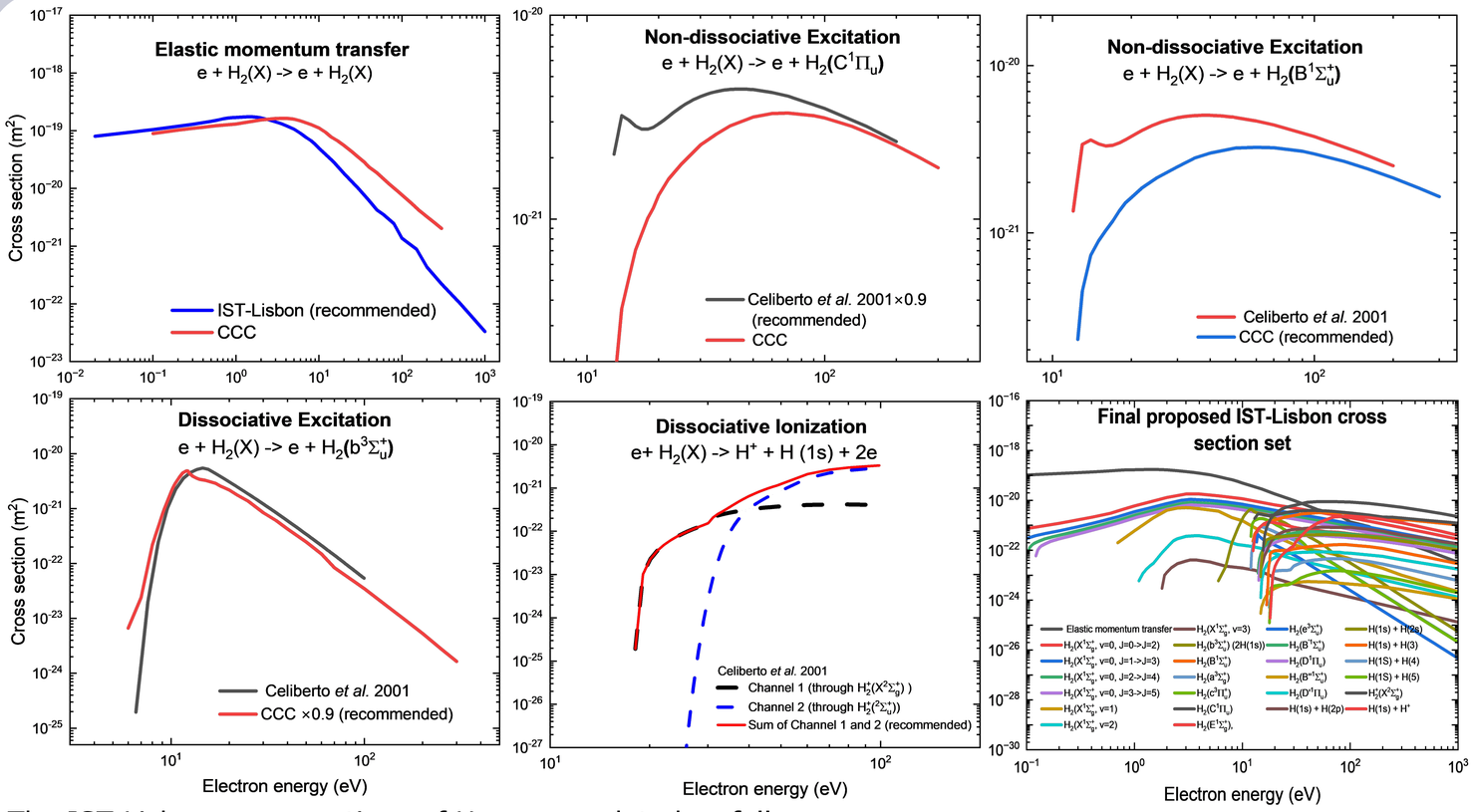
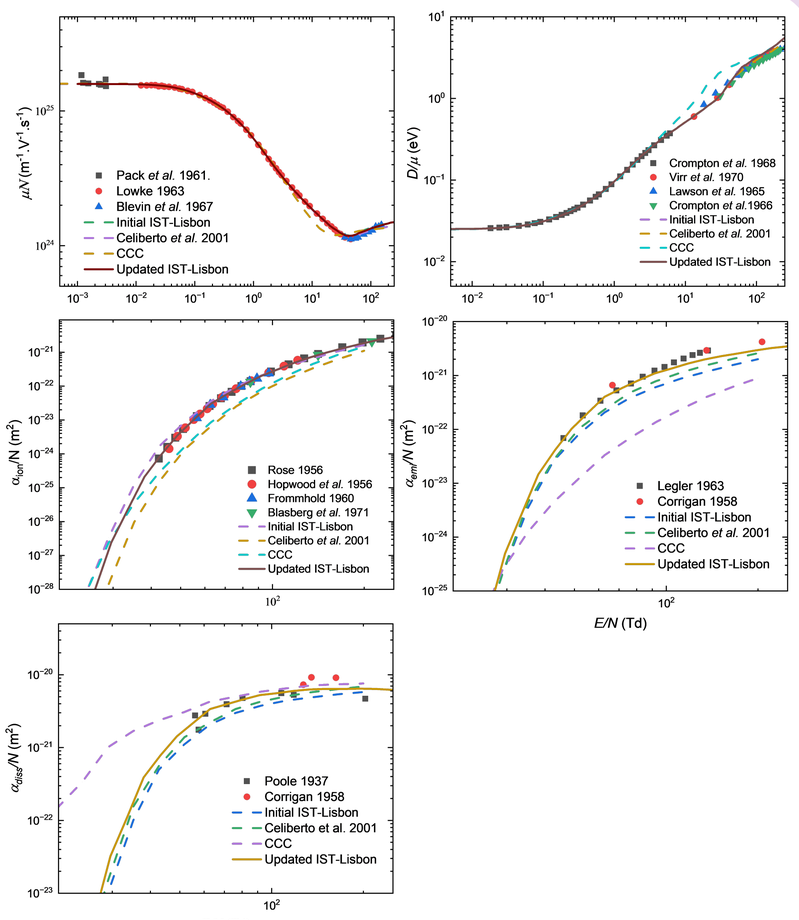
Introduction

The efficient modelling of N_2-H_2 plasmas is key to understand the main kinetic pathways leading to **plasma assisted synthesis and decomposition of NH_3** [1]. In low-temperature plasmas, electron collisions with atomic/molecular neutral-species are one of the most important kinetics mechanisms, and therefore **complete and consistent sets of electron-neutral collisional cross-sections** are essential data for plasma modelling [2].
In this work,
(i) we update the **electron-impact cross section set for ground-state H_2** published in the IST-Lisbon database of the LXCat open-access website [3];
(ii) we propose an **electron-impact cross section set for ground-state NH_3**.
The swarm analysis was carried out using the LisbOn KInetics Boltzmann solver (LoKI-B) [4], to calculate electron transport parameters (reduced mobility or drift velocity, reduced diffusion coefficient, characteristic energy) as well as several reduced Townsend coefficients (ionization, dissociation, emission, attachment).

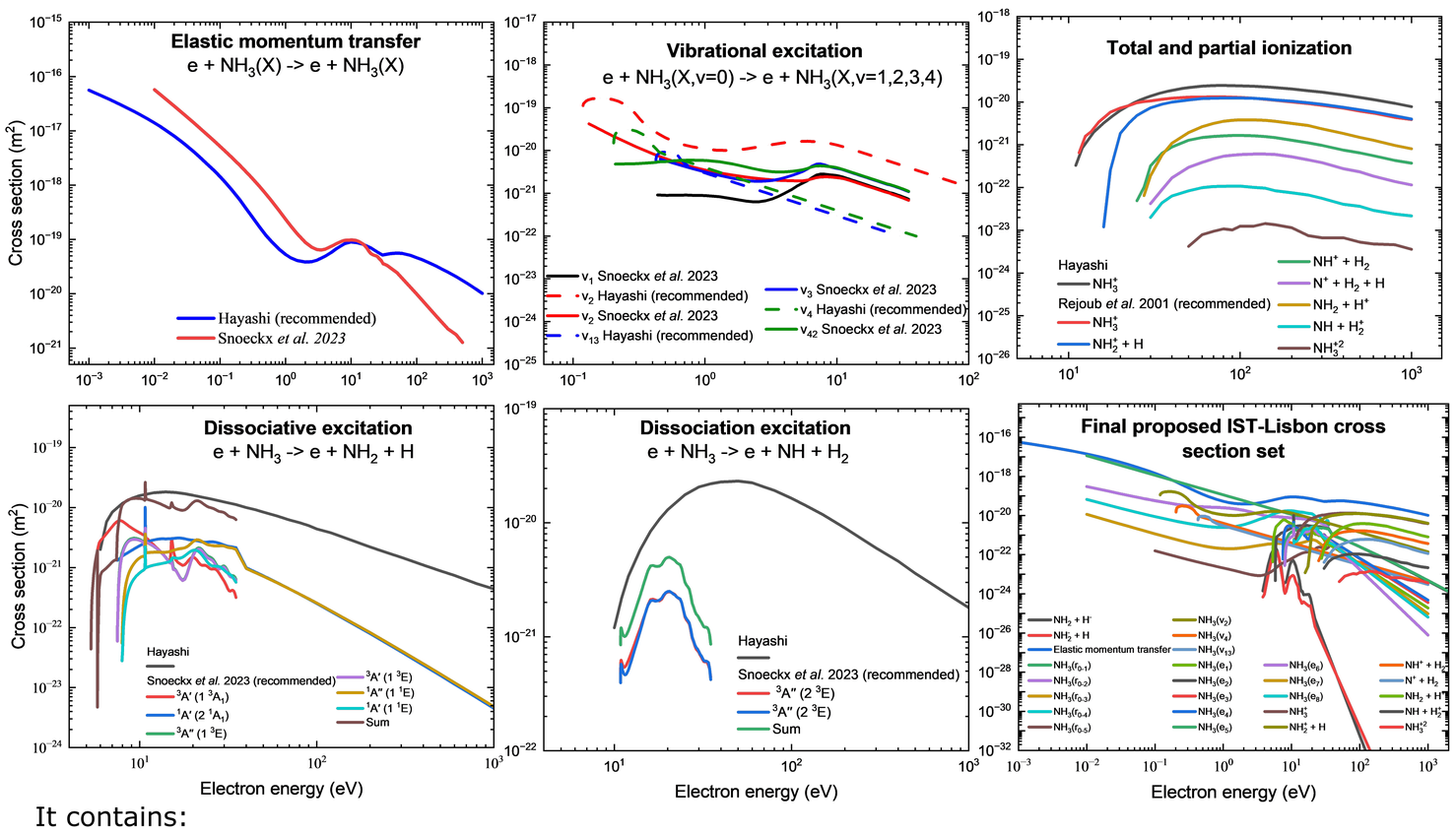
Cross sections of H_2 and swarm analysis

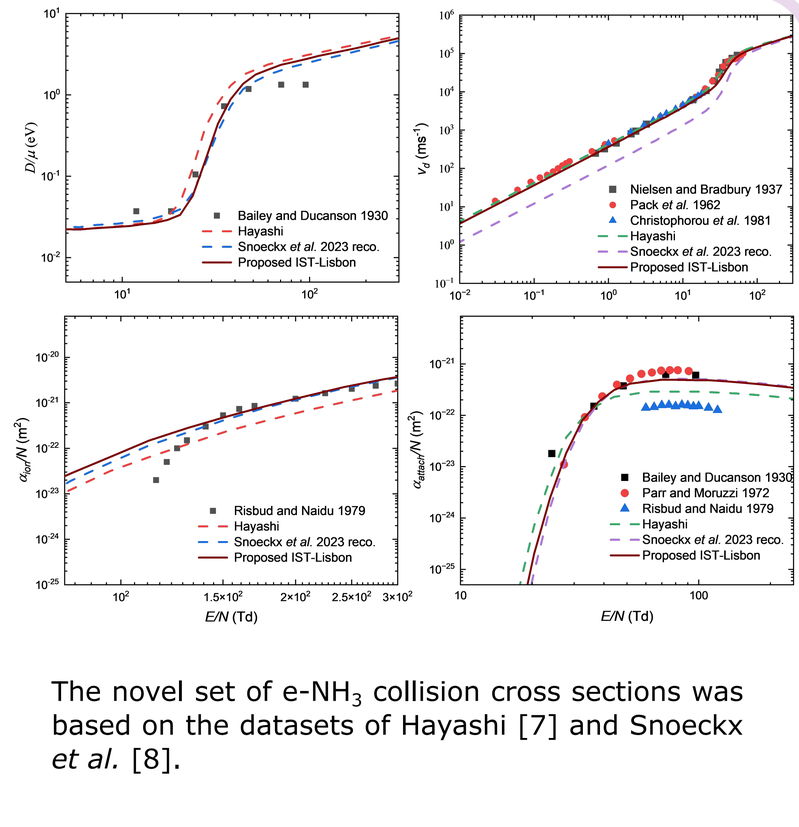




The IST-Lisbon cross-sections of H_2 were updated as follows:
(i) the excitation cross section to $b^3\Sigma_u$ was replaced with CCC [5], scaled by a factor of 0.9;
(ii) the excitation to $B^1\Sigma_u$ was adopted from CCC [5];
(iii) the excitation to $C^1\Pi_u$ was adopted from Celiberto et al. [6] scaled by a factor of 0.9;
(iv) the dissociative ionization cross section was updated by summing the two dissociative channels reported by Celiberto *et al.* [6].

Cross sections of NH_3 and swarm analysis





The novel set of e-NH_3 collision cross sections was based on the datasets of Hayashi [7] and Snoeckx *et al.* [8].

It contains:
(i) elastic momentum-transfer and vibrational cross sections from Hayashi [7]
(ii) rotational and electronic excitation cross sections calculated by Snoeckx *et al.* [8]
(iii) dissociative electron attachment cross section measured by Rawat *et al.* [9]
(iv) total and partial ionization cross sections measured by Rejoub *et al.* [10]

Final remarks

Both sets of cross sections are **complete and consistent**, because they include the most relevant mechanisms for the electron-neutral exchange of energy and momentum, and because when used in a two-term electron Boltzmann solver they predict **swarm parameters in agreement with experimental measurements** [11], within less than 15%.

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