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Rate coefficients for H_2^+ ions in Ar gas

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Goal

In this paper we show predictions for the low energy cross sections and transport properties for the H_2^+ in Ar gas. These data are needed for modelling in numerous applications of technologically important. A Monte Carlo simulation method is applied to accurately calculate transport parameters for the hydrodynamic regime. We discuss new data for H_2^+ ions in Ar gas where the mean energy, drift velocity, flux and bulk values of reduced mobility and rate coefficients are given as a function of low and moderate reduced electric fields, E/N (E-electric field strength, N-gas number density).

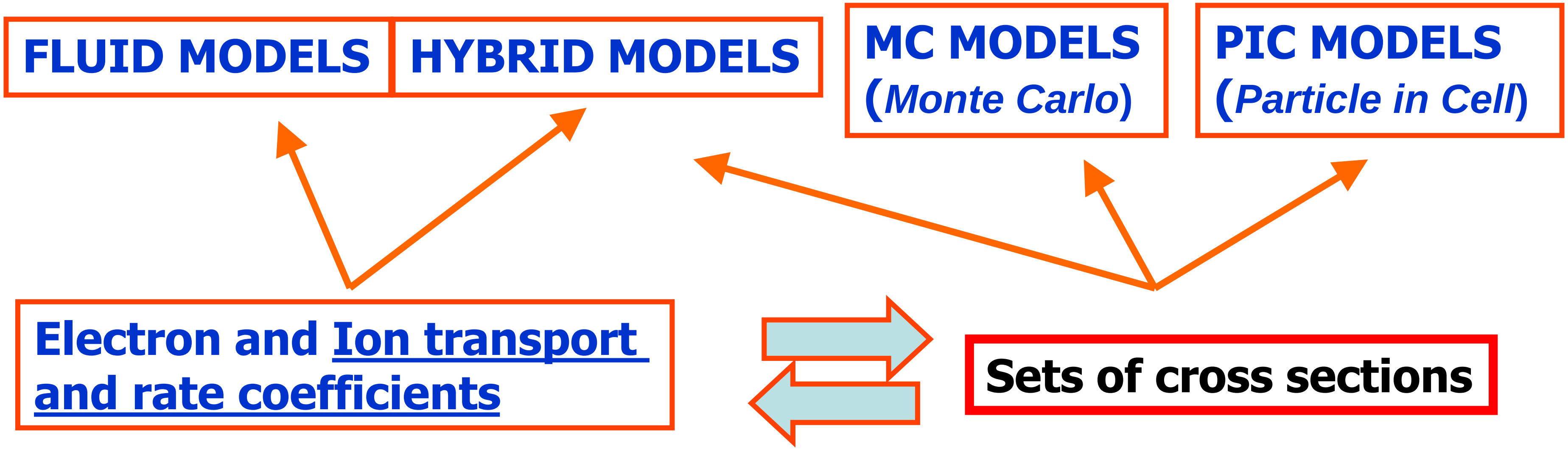
Introduction

- Ion charge transfer reactions with molecules are unavoidable elementary processes in modeling kinetics in terrestrial, industrial and astrophysical plasma in the detection of dark matter.
- Motivational factors for this study have been identified and this paper reports on a topic important for both basic studies and application.

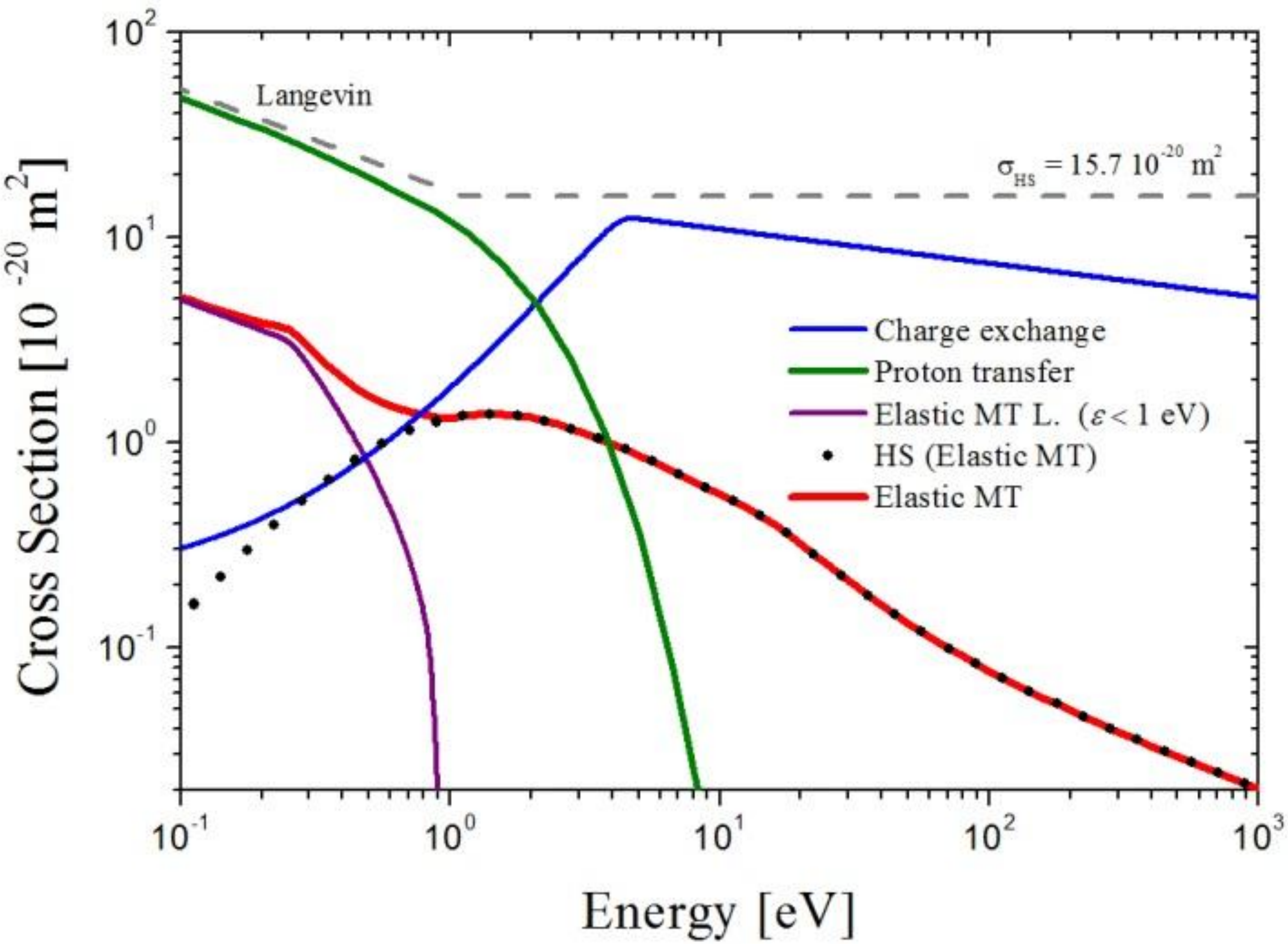
- Transport properties needed for modeling H_2 discharges containing H_2^+ ions are calculated by the Monte Carlo method.

For collisions of H_2^+ ions with H_2 molecules, at energies below 1 eV, the total cross-section is labeled as 'Langevin' in Figure 1 and includes anisotropic forward scatterings, an isotropic capture part, rotational excitations, as well as the charge exchange reaction. The transition from Langevin's cross-section to the collision of rigid spheres (labeled as σHS in the figure) occurs at energies around 1 eV.

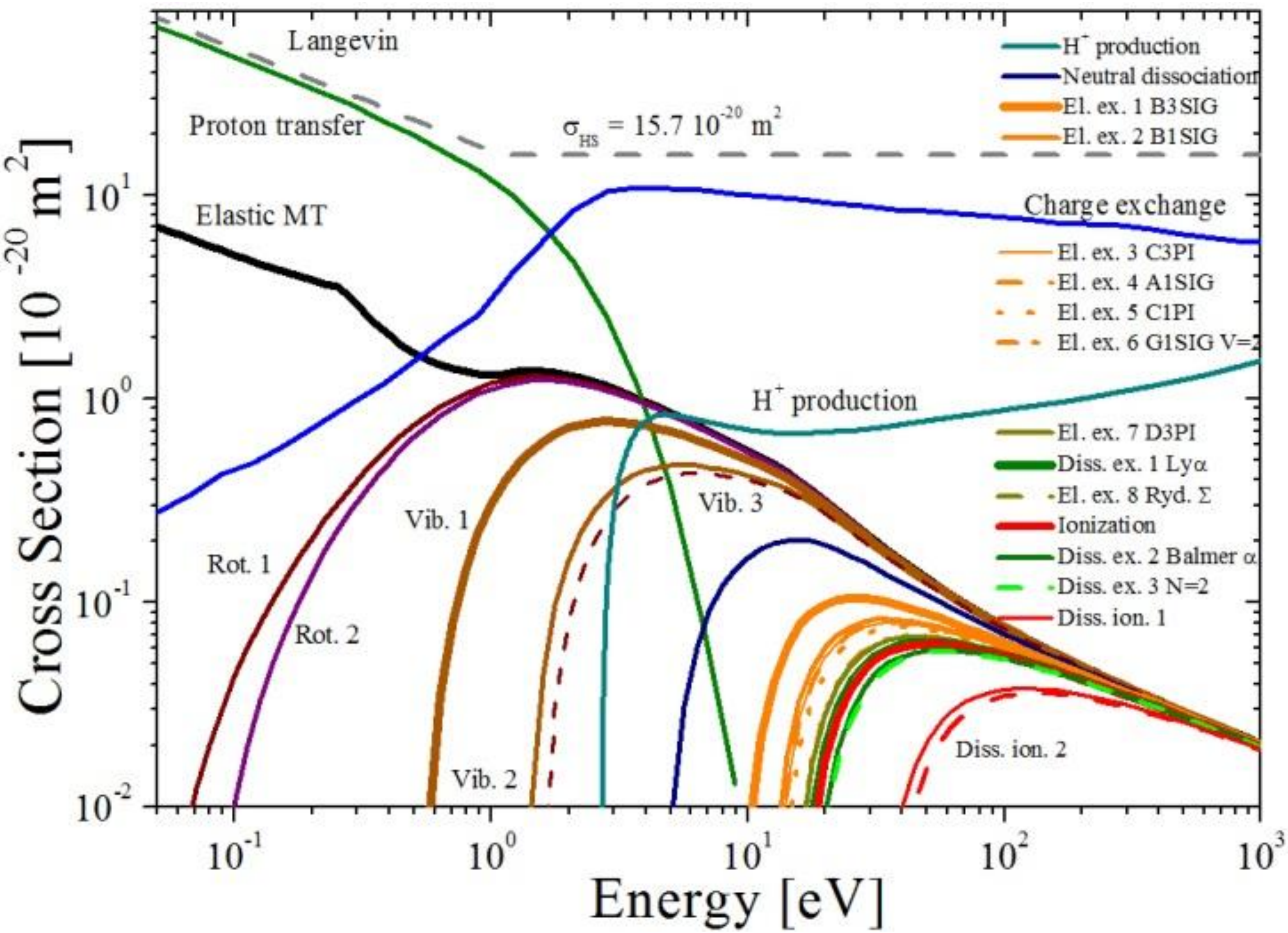
In Figure 3 we present cross sections for collisions of H_2^+ with Ar versus laboratory energy of H_2^+ of Ar. The symbols and collisional processes are: Ar H^+, proton transfer to Ar H^+; Ar^+ plus fast H_2, charge transfer to form Ar^+ and fast H_2; H^+; dissociation to form H^+; Lyman Alfa radiation; and e, production of electrons and ionization.



Calculated cross sections will be taken as basis for interpretation and modeling of electron kinetics plasma applications.
Calculation of rate coefficients in DC fields by Monte Carlo simulations.



•**Figure 1.** Elastic momentum transfer cross section for collisions between H_2^+ ions and H_2 molecules as a function of collision energy.



•**Figure 2.** Complete set of cross sections for ion (H_2^+) and molecule (H_2) interactions

• as a function of collision energy.

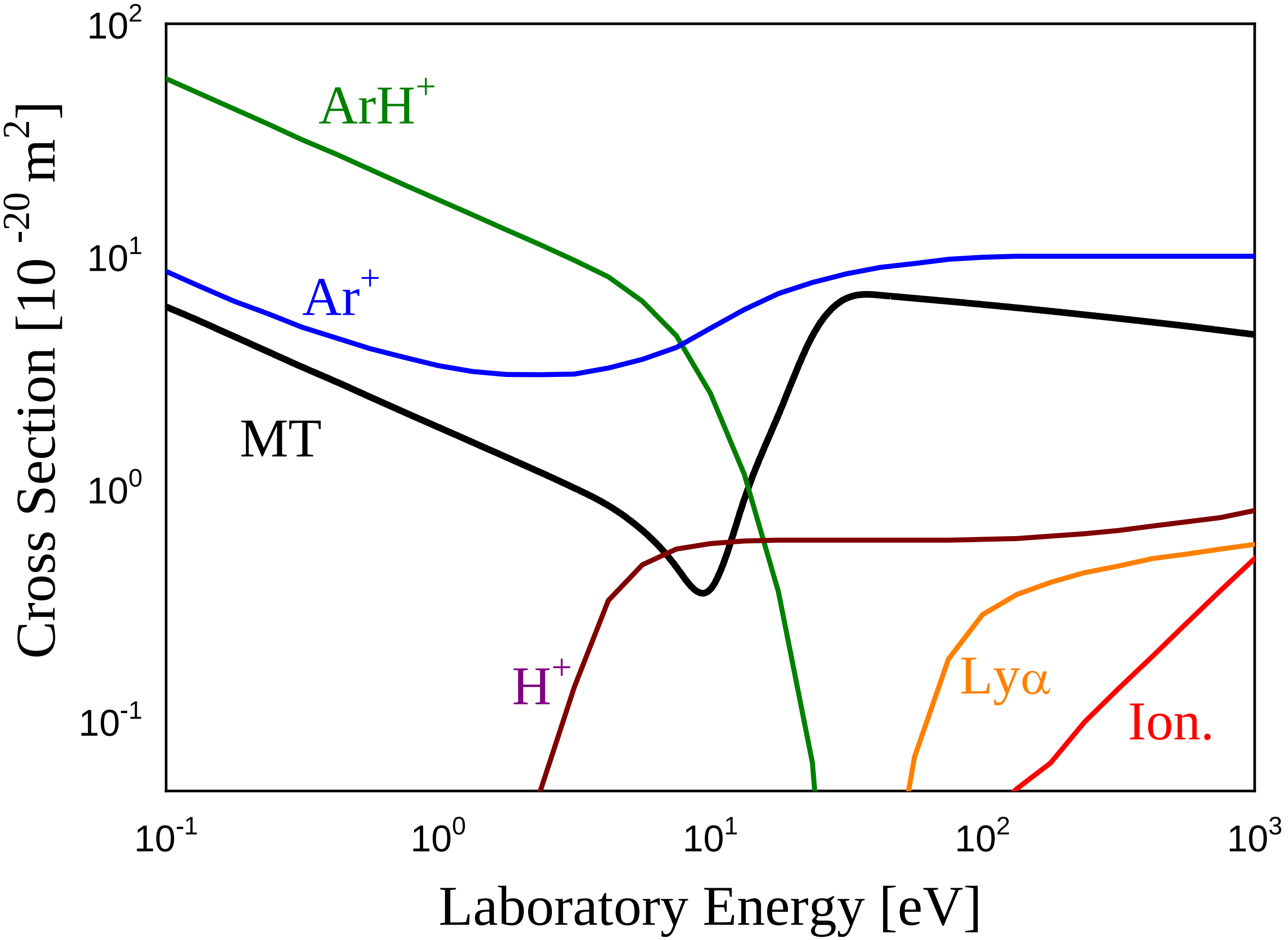


Figure 3. Cross section set for H_2^+ in Ar.

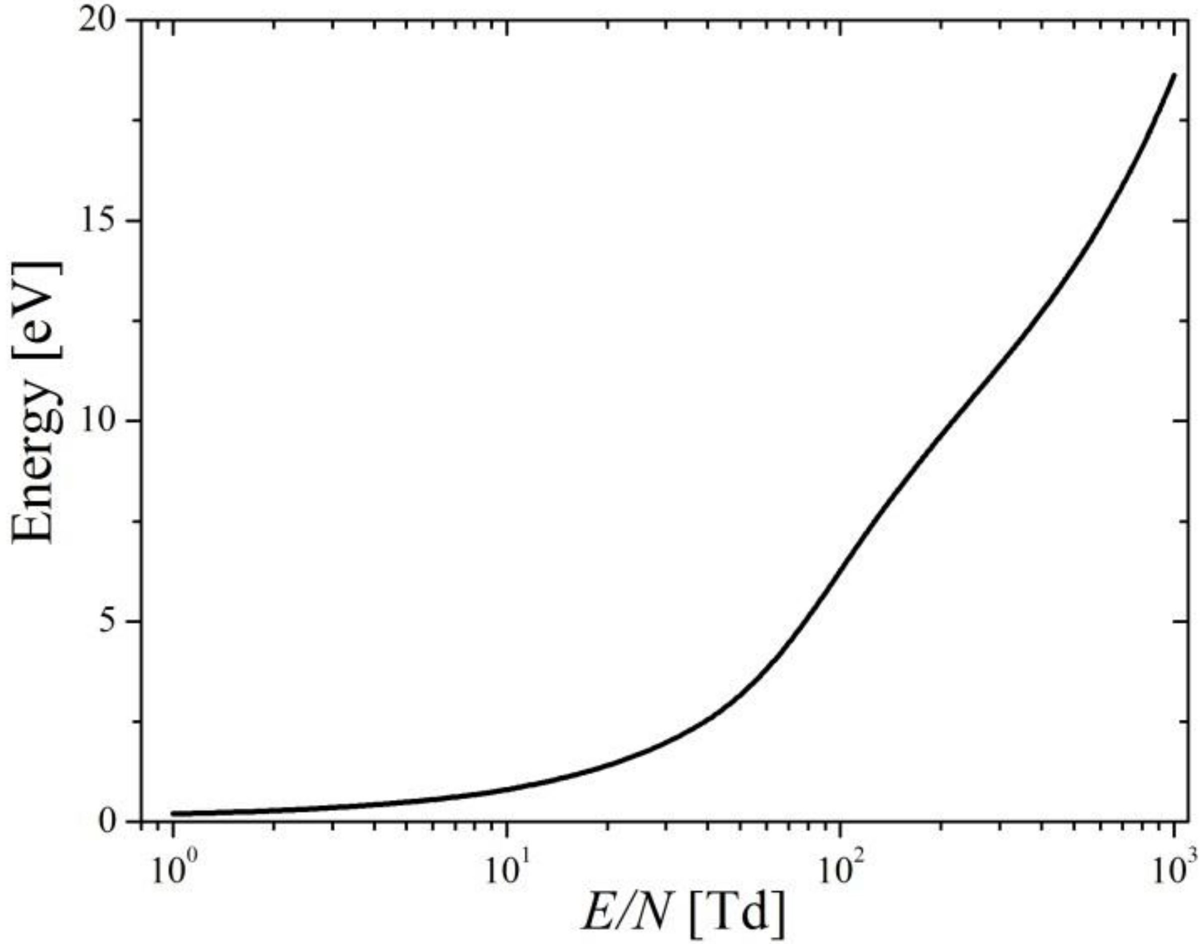


Figure 4. Mean energy as a function *E/N* for H_2^+ in Ar.

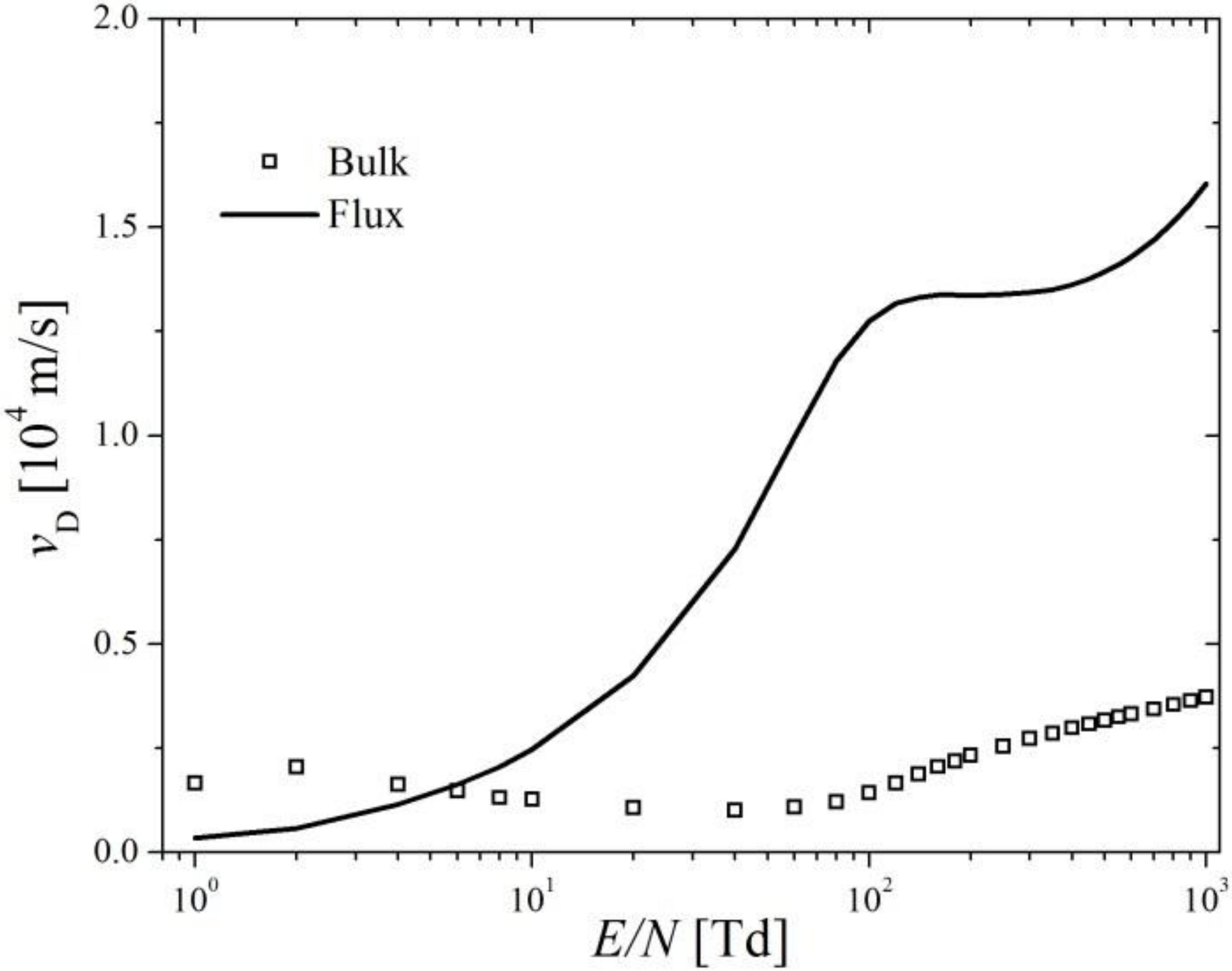


Figure 5. Drift velocity as a function *E/N* for H_2^+ in Ar.

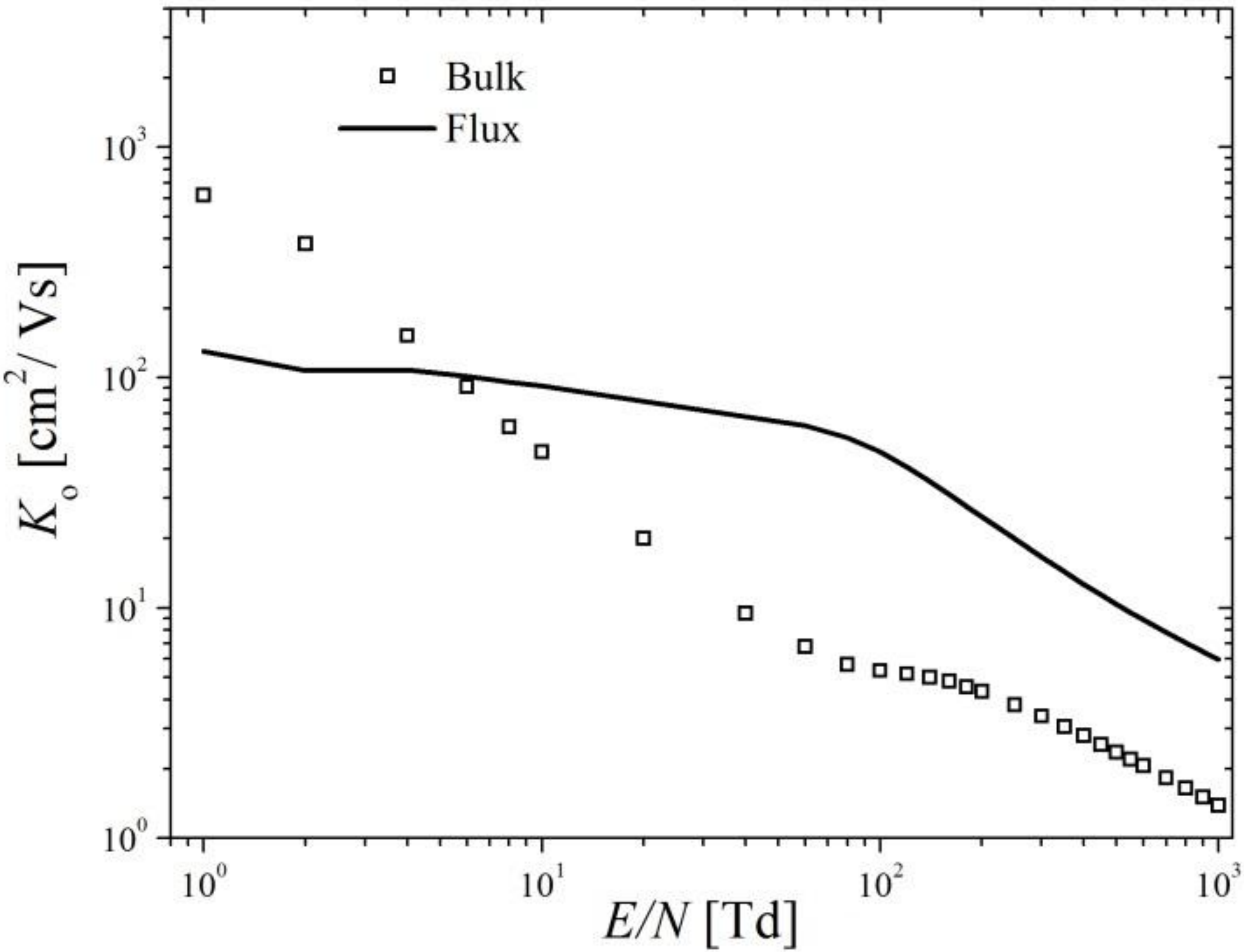


Figure 6. Bulk and flux reduced mobility for H_2^+ in Ar a function of *E/N* at 300 K.

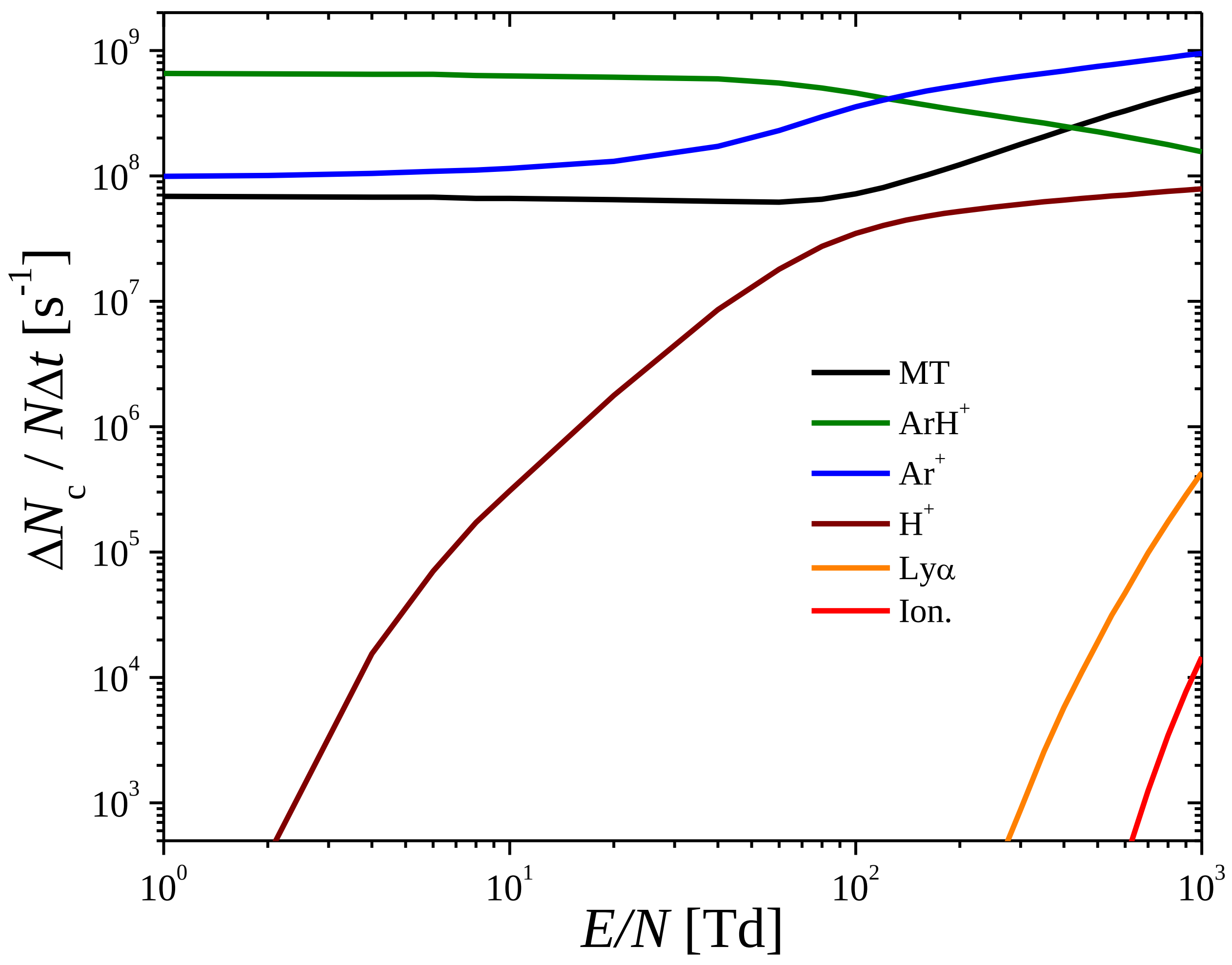


Figure 7. Rate coefficients as a function *E*/*N* for H_2^+ in Ar.

Conclusion

- The Monte Carlo technique was applied to carry out calculations of the mean energy, drift velocity, bulk and flux reduced mobility and rate coefficients as a function of reduced DC electric field. The results are believed to be a good base for modeling, which could be further improved when measured values of transport coefficients become available and then we could perform this analysis again.

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