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

## <u>Maik Budde<sup>1,2\*</sup></u>, Tiago Cunha Dias<sup>2</sup>, Tiago Silva<sup>2</sup>, Luca Vialetto<sup>3</sup>, Nuno Pinhão<sup>2</sup>, Vasco Guerra<sup>2</sup>

<sup>1</sup> Department of Applied Physics, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands
<sup>2</sup> Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa, Portugal
<sup>3</sup> Theoretical Electrical Engineering, Faculty of Engineering, Kiel University, Kaiserstraße 2, 24143 Kiel,

Germany

\*corresponding author e-mail: <u>m.budde@tue.nl</u>

Select: poster presentation

In vacuum science, there is no way around water as it is an omnipresent impurity that is frequently encountered in many applications. Others might deliberately add it to their system, e.g. in CO<sub>2</sub> plasma conversion to use water as an abundant hydrogen source. In these applications, the interaction of water molecules with electrons is crucial. A common description of the electron kinetics is the solution of the electron Boltzmann equation in the two-term approximation yielding the electron energy distribution function. However, for water the required complete and consistent set of electron collision cross sections is not 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 considering the anisotropy of the scattering process [1,2]. The set is shown in fig. 1 and is validated against experimental electron swarm parameters like drift velocity, Townsend coefficient etc. and will be made available in the IST-Lisbon database with LXCat [3].



Figure 1: Electron collision cross sections with water molecules  $\sigma$  against the electron energy  $\epsilon$ . Nonconservative collisions cause changes in electron number due to ionization or attachment.

This work was partially supported by the European Union's Horizon 2020 research and innovation programme under grant agreement MSCA ITN 813393, and by Portuguese FCT-Fundação para a Ciência e a Tecnologia, under projects UIDB/50010/2020, UIDP/50010/2020 and PTDC/FIS-PLA/1616/2021 (PARADiSE)

## References

[1] Itikawa, Rotational Transition in an Asymmetric-Top Molecule by Electron Collision: Applications to  $H_2O$  and  $H_2CO$ , J. Phys. Soc. Jpn. 32 (1972) 217-226

[2] Vialetto et al., Effect of anisotropic scattering for rotational collisions on electron transport parameters in CO, Plasma Sources Sci. Technol. 30 (2021) 075001

[3] Alves, The IST-LISBON database on LXCat, J. Phys.: Conf. Ser. 565 (2014) 012007