Publ. Astron. Obs. Belgrade No. 103 (2024), 100 *Invited Lecture*
https://doi.org/10.69646/aob103p100

LXCAT 3 AND BEYOND – FOSTERING REPRODUCIBILITY IN LOW-TEMPERATURE PLASMA SCIENCE

JAN VAN DIJK and DAAN BOER

Elementary Processes in Gas Discharges, Department of Applied Physics and Science Education, Eindhoven University of Technology, The Netherlands
E-mail j.v.dijk@tue.nl, d.j.boer@tue.nl

Abstract. The LXCat project (Pitchford et al. 2017, Carbone et al. 2021) provides electron-impact cross sections, swarm parameters, interaction potentials and other data that are required for low-temperature plasma (LTP) modeling and simulation. It is a community-driven project that contains approximately 30 000 cross sections, and welcomes in the order of 40 000 visitors per year. Version 2 of the website can be found at https://lxcat.net/home/. In spite of its success, a number of issues have been identified in recent years that stand in the way of further progress (sec. 6, 7 of Carbone et al. 2021). These concern the data format, the choice for the (SQL) database and the design of the software stack.

In this contribution, the authors report on the status of "LXCat 3". This new version of the LXCat database is scheduled to be made available to the general public in September 2024 and addresses all of the above-mentioned concerns. It is based on a standard (JSON) file format that is underpinned by a well-defined data model that is encoded in JSON-Schema, it uses the multi-model ArangoDB database and features a design that allows interaction with the data other than through the LXCat website. LXCat3 is free software, available from the Github repository https://github.com/LXCat-project/LXCat. Special attention has been paid to a proper versioning of data items and combinations thereof, and references to particular data can now be made unambiguously using so-called "permalinks". This feature will have a great impact on the reproducibility of studies in LTP science, especially when complex mixtures of molecular gases are involved and the input data needs are excessive.

After an introduction to the LXCat project and a discussion of the features of LXCat3, live demonstrations of the new platform will be given. The presentation will conclude with a discussion of recent developments, in particular the application of the framework to full plasma chemistries, including non-electronic processes.

References

Carbone E.A.D. et al.: 2021, *Atoms* **9**, 16, https://doi.org/10.3390/atoms9010016
Pitchford L.C. et al. : 2017, *Plasma Processes and Polymers*, **14**, 1600098, https://doi.org/10.1002/ppap.201600098