



Data input for modelling non-equilibrium low temperature discharges: the LXCat project

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The LxCat project (2009 - present)

LxCat (ELECtron (and ion) SCATtering): a community-based project for storing, sharing, and evaluating data needed to model non-equilibrium low temperature plasmas.

Electron + neutral cross sections / oscillator strengths/ swarm parameters

Ion + neutral cross sections / interaction potentials / swarm parameters

Plasma-surface interactions

Plasma chemistry

Radiation

Modeling charged particles generation & transport



LEVEL OF DESCRIPTION

KINETIC MODELS

$f(r,v,t)$ distributions
(Boltzmann or Monte Carlo simulations)

HYBRID MODELS

FLUID MODELS

(macroscopic quantities)

DATA NEEDS

Electron- and ion-neutral
scattering cross sections

“Complete” sets of electron/ion - neutral cross sections

Certain aspects of ion or electron behavior are treated with particle models; other aspects with fluid models.

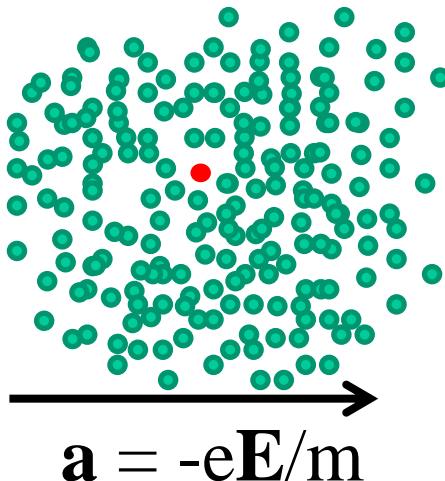
Swarm parameters: electron and ion transport coefficients → mobility and diffusion coefficients, ionization rates,...

Boltzmann transport equation



The **Boltzmann** transport **equation** allow to describe the statistical behavior of a system not in a state of equilibrium. Parametrization versus: E/N, gas composition, angular frequency of the external field, B field.

$f(r, v, t)$ = velocity probability distribution function



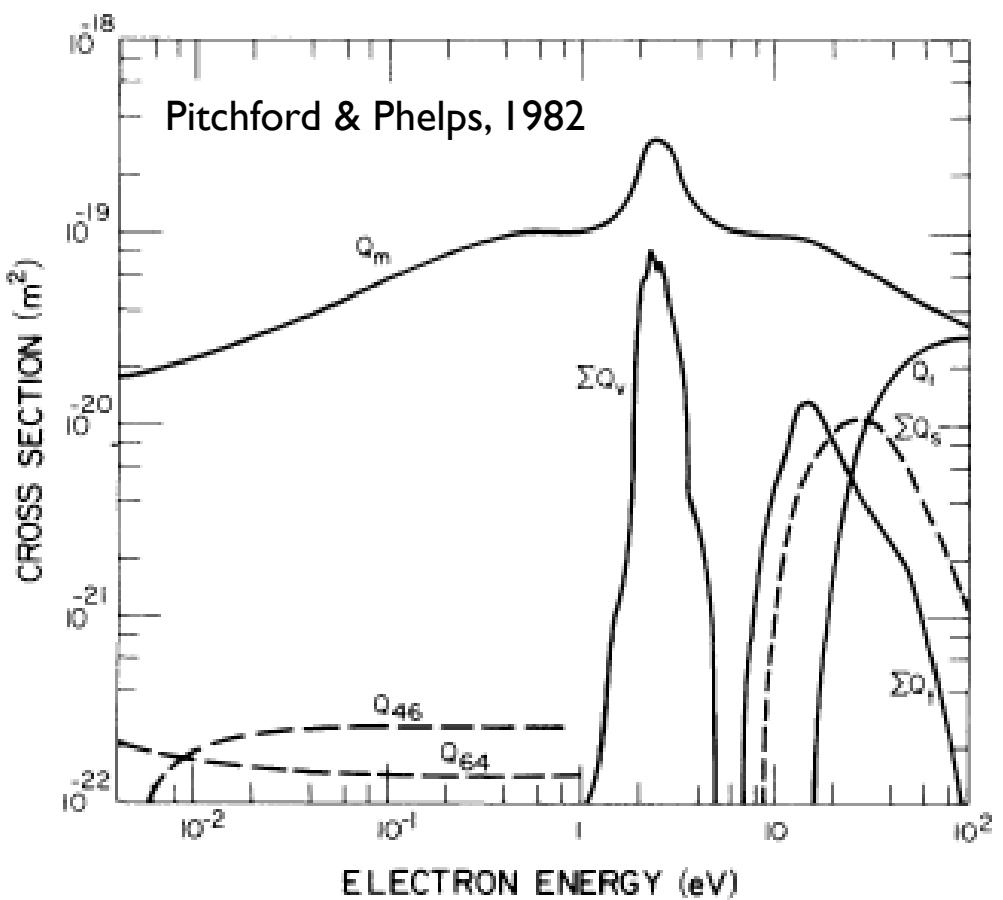
$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f + \vec{a} \cdot \nabla f = NC[f]$$

↖ ↘ ↗
transport in r transport in v Collisions

where $\int f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v} = n_e(\mathbf{r}, t)$

e-/ion transport & rate coefficients are integrals over $f(r, v, t)$.

Input data for solving the Boltzmann equation



Types of collisions:

- **Elastic**

Recoil energy loss, momentum transfer ($Q_{m,\text{el}}$)

- **Inelastic**

Discrete energy losses due to excitation of rotational, vibrational and electronic states ($Q_{k,T}$)

- **Ionization**

Two electrons exit the collision event ($Q_{i,T}$, energy sharing)

- **Attachment**

An electron is lost after collision with a neutral species.

Complete sets of e-/neutral cross sections available on



....for electron scattering in **COLD gases**

Definition: A complete set of cross sections consists of elastic momentum transfer, and total cross sections for the processes of ionization, attachment and excitation. Complete sets of cross sections are needed as input to a Boltzmann equation solver to determine the electron or ion energy distribution function.

Atomic gases

Ar, C, Cu, H, He, Hg, Kr, Mg, N, Ne, Na, O, Xe

Diatom gases

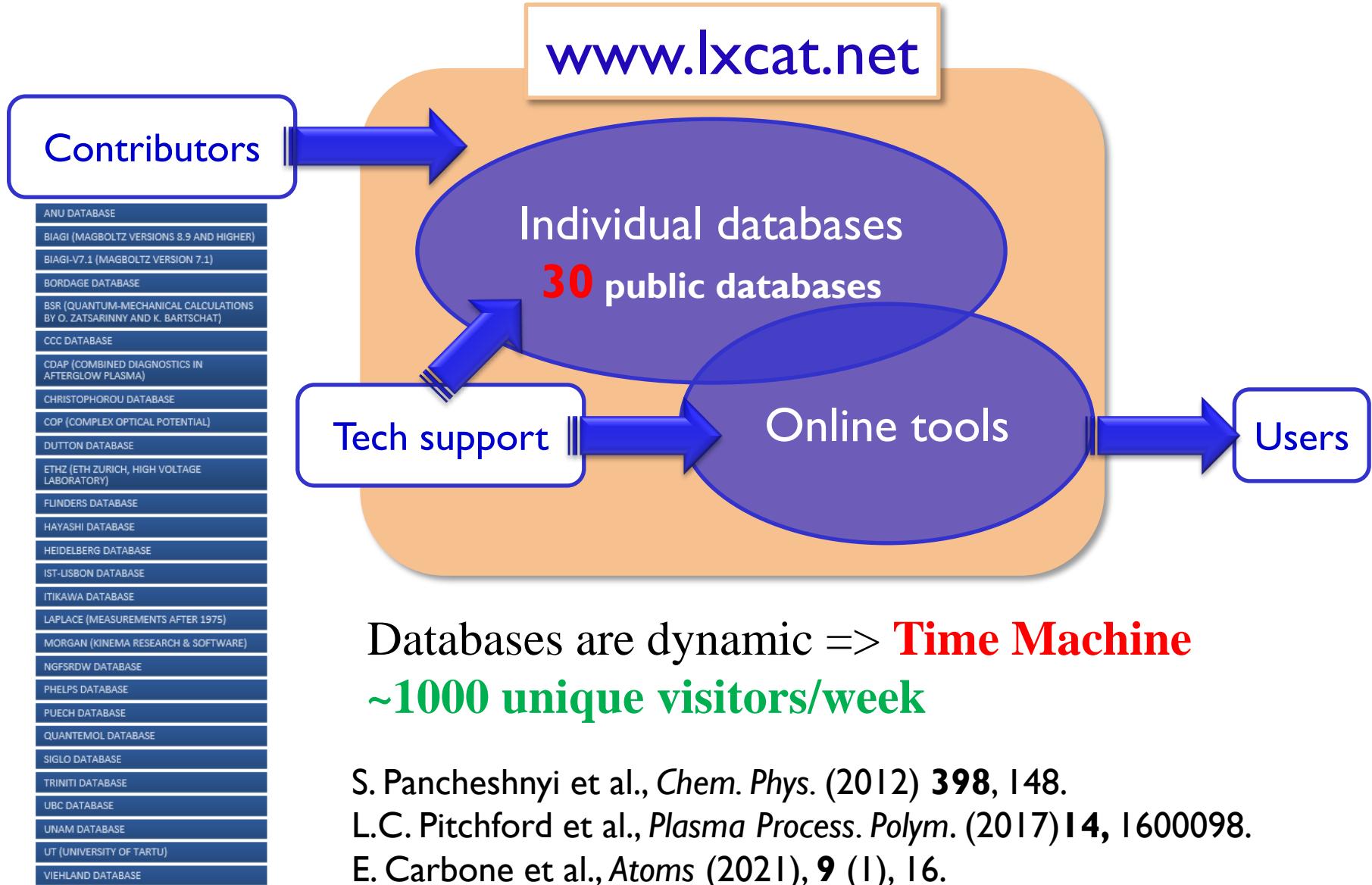
CH, CO, Cl₂, D₂, F₂, H₂, HCl, N₂, NO, O₂

Polyatomic gases

C₂H₂, C₂H₄, C₂H₆, C₃H₆, C₃H₈, CCl₂F₂, CCl₄, CF₄, CH₄, CH₃, CH₄, CHF₃, CO₂, H₂O, N₂O, SF₆, SO₂, Si₂H₆, Si(CH₃)₄, SiH₄



LXCat structure – databases & online tools

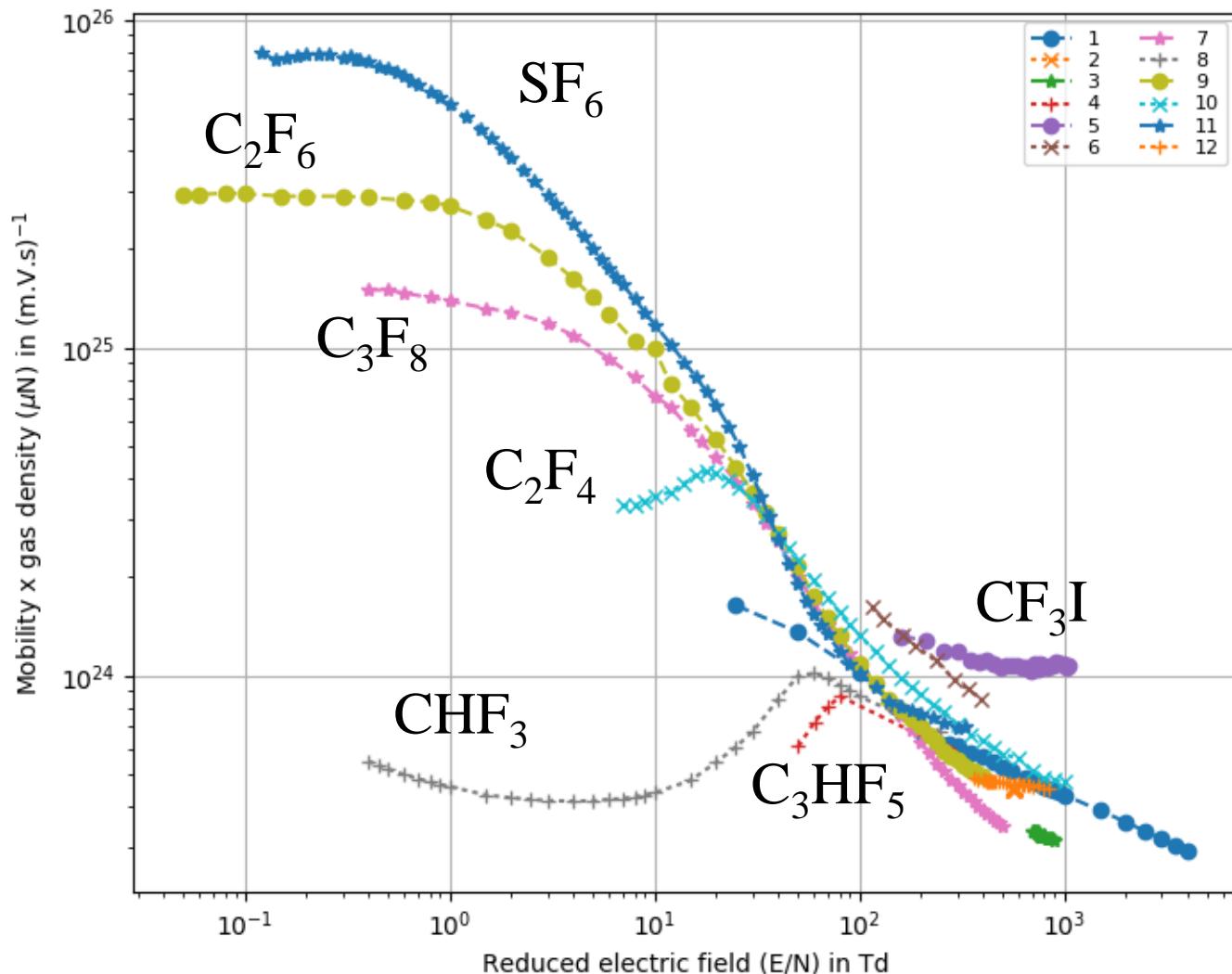


What can be done on LXCat ?

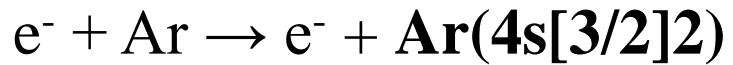


- 1) **Look up for cross section data:** theoretical and experimental dataset of electron and ion collisions with neutrals
- 2) **Find numerized measurements from swarm experiments**
- 3) **Online calculations using BOLSIG+**
- 4) **Online comparison** of swarm measurements and calculated parameters using scattering cross sections datasets
- 5) Discuss and ask for advice (Google group)

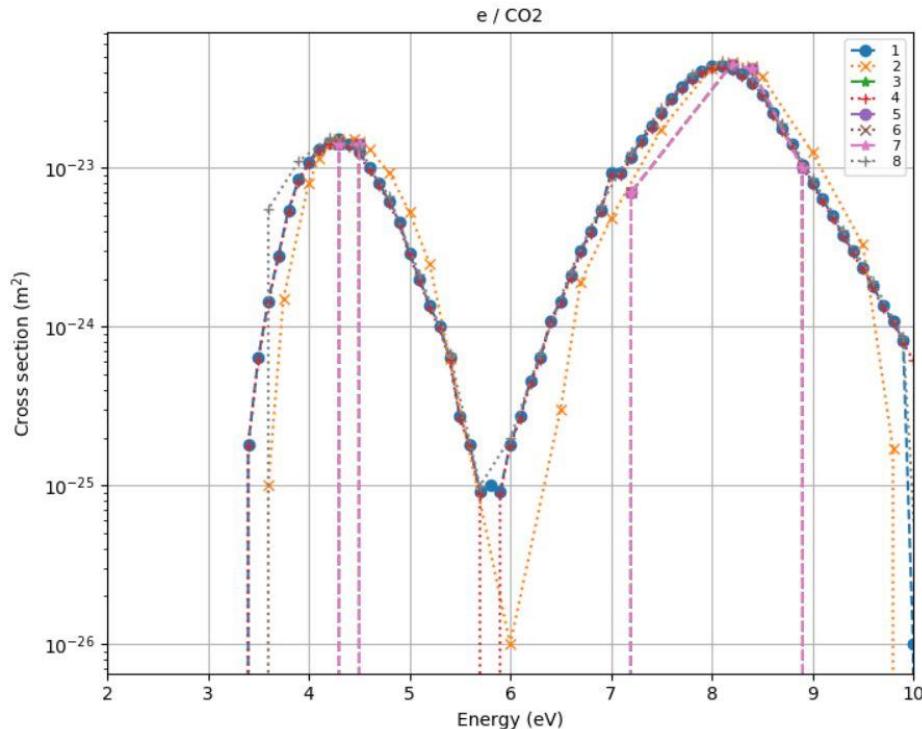
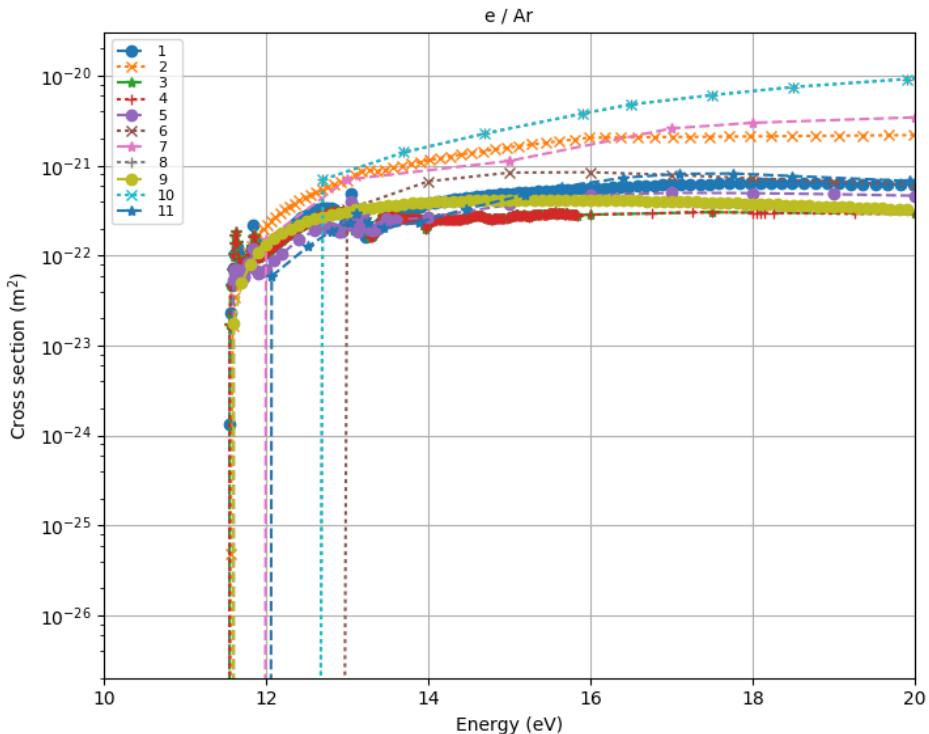
Comparison of data: electron mobility



Comparison of data: cross sections

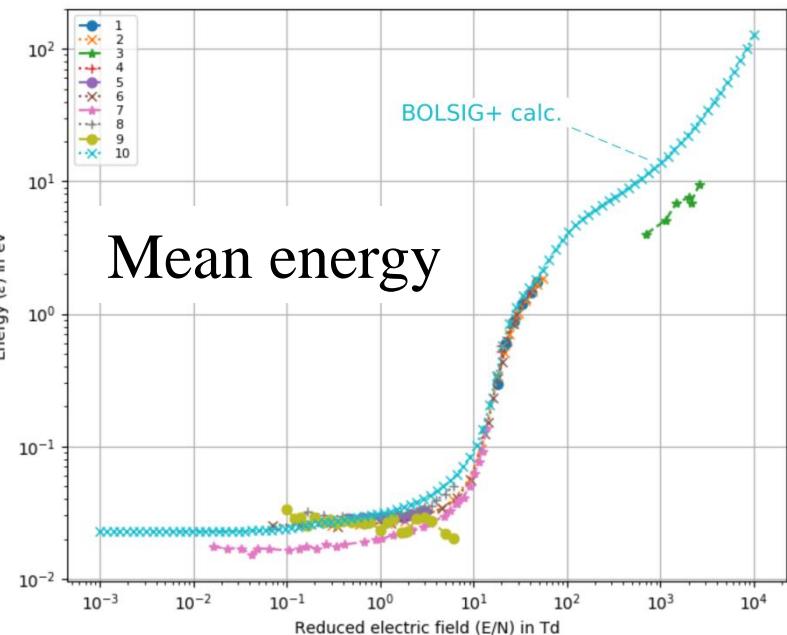
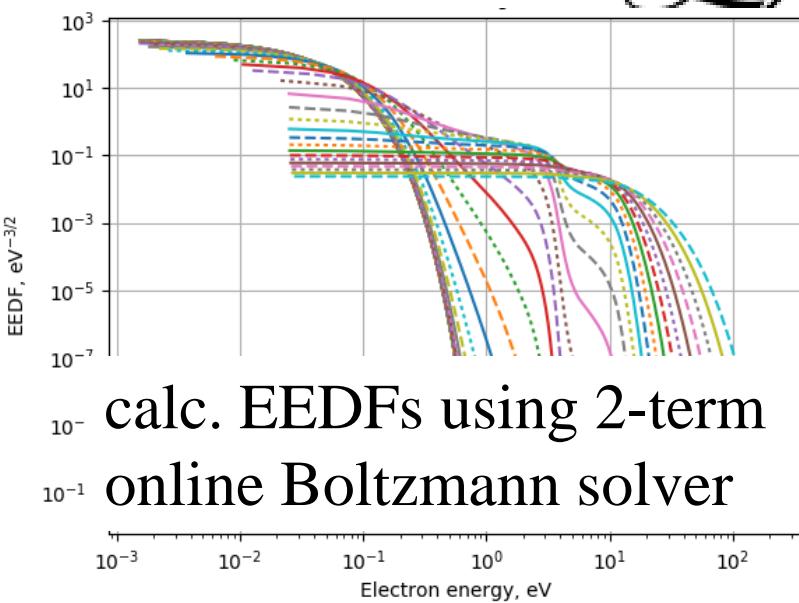
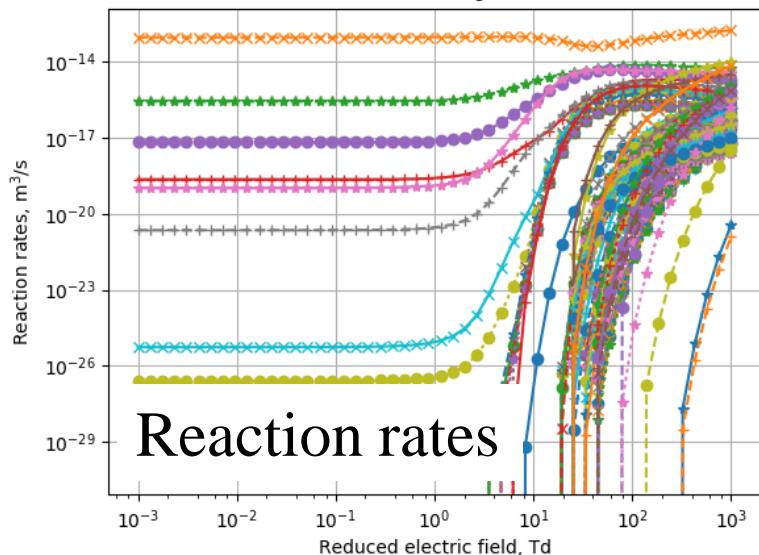
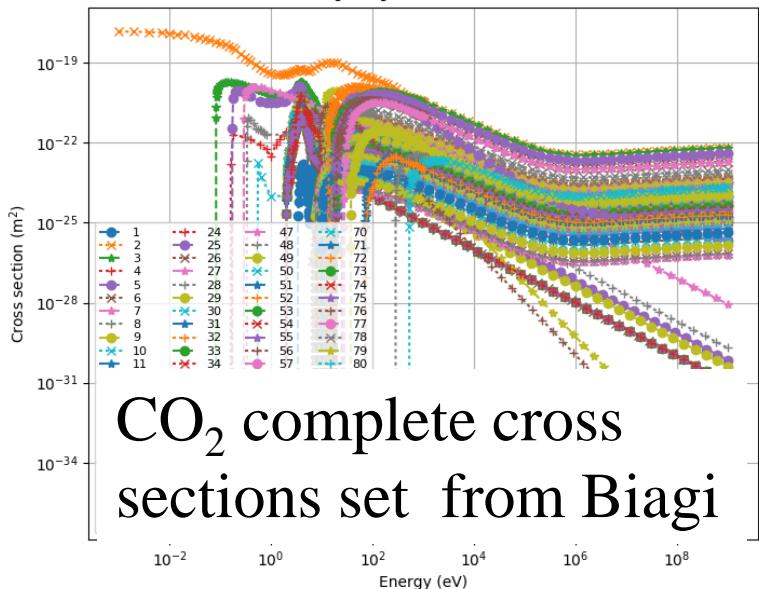


Electron attachment to CO_2

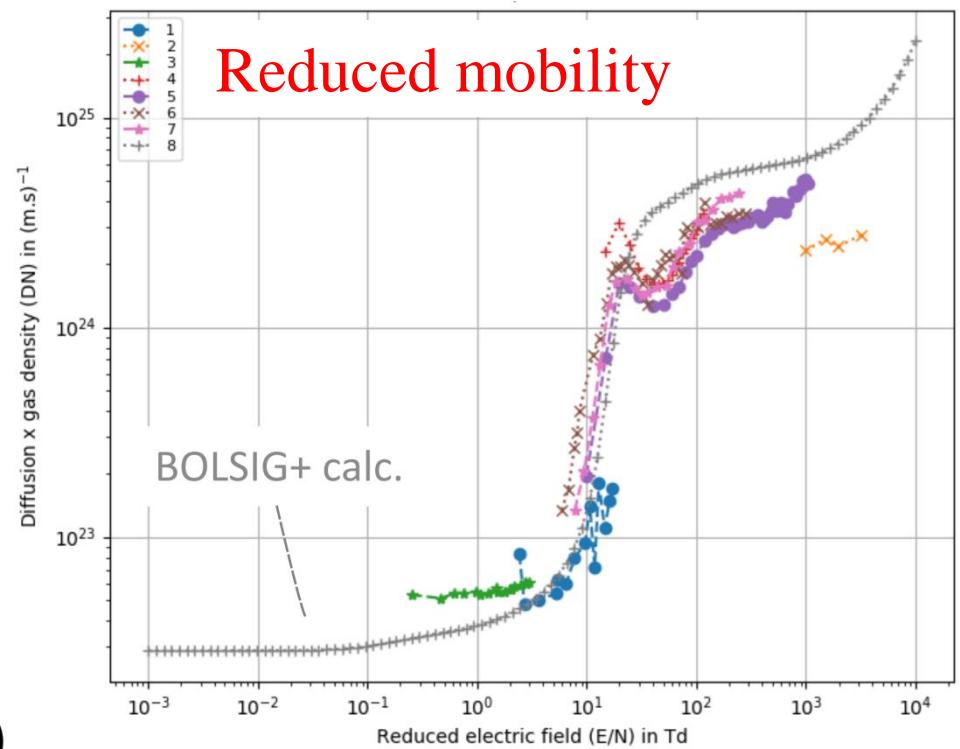


- Comparison between different databases can be done online.
- Very good agreement in some cases: it does NOT always mean better known cross sections (check origin of data and measurement/calculation methods).

Calculation of swarm parameters (0.001-1000 Td)



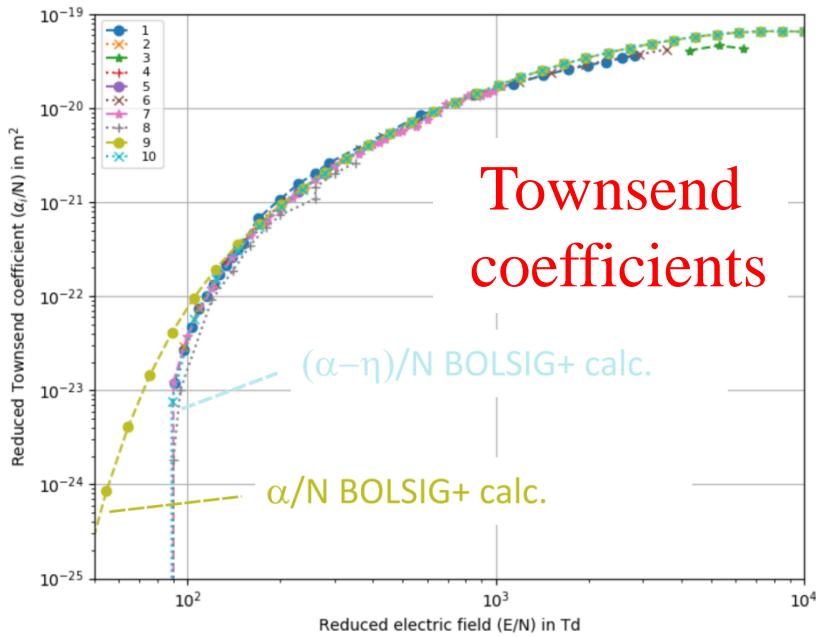
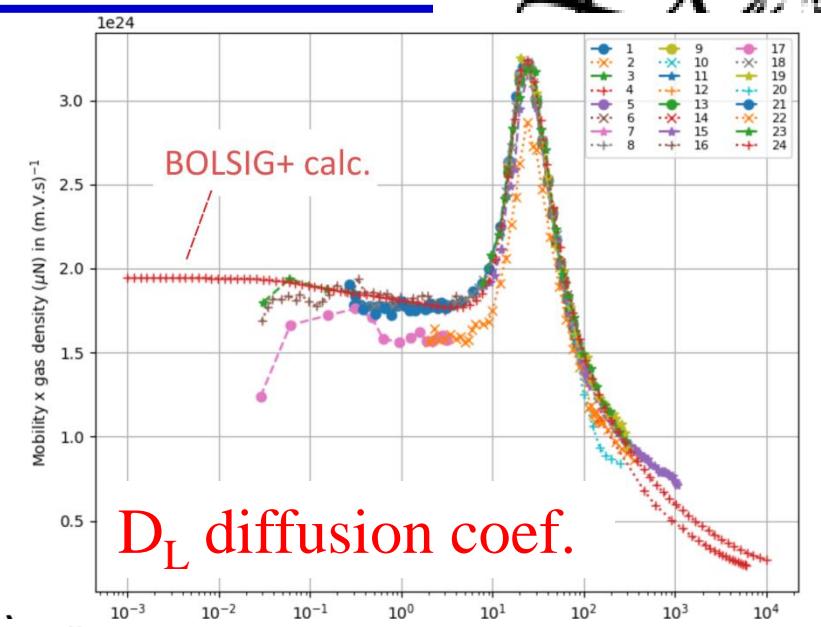
Comparison with measured transport parameters



Calculated transport coefficients for pure CO_2 using Biagi database versus experiments

$$\text{E}/\text{N} = 0.001 - 10000 \text{ Td}$$

$$(1 \text{ Td} = 10^{-21} \text{ V m}^2)$$



LXCat policy



- 1) Anyone willing to contribute data to the site can request a password and set up a database. => Data for the same processes can be listed in multiple databases. **LXCat does not recommend data** (see discussion in E Carbone et al., Atoms (2021), 1, 16).
- 2) The website is **open access** and data can be downloaded without registering or paying a fee, but **proper referencing is essential** for the survival of LXCat.

Required reference format:

[database name], www.lxcat.net, [retrieval date]

+ List all references given in the database for the species

3. **Databases are dynamic.** Contributors make changes as new data become available or when corrections are needed. **Time machine** allows retrieving database at any given time in the past.

Some additional comments for discussion



- 1) How to link swarm data with parameters relevant to the gas detectors community?
- 2) Gas temperature effects on swarm data (e.g. effect of rotational distribution function on energy and momentum losses)
- 3) Pressure dependence for 3-body (attachment) processes
- 4) Possibility to host new data types
- 5) ...

LXCat challenges and outlook



- **Sustainability:** LXCat is a volunteer project
 - Long term future of the project
 - Maintenance of web infrastructures
- **Transcription** of data from literature: community needs ?
- **Handling (very) large state to state** datasets: structure, notation, re-scaling,...
- Hosting new types of data ?
- Developing additional **vizualization, data analysis** tools

Financial support of the project via donations to the **Data for Plasma Modelling non-profit association** is now possible.

More information and contact



Review

Data Needs for Modeling Low-Temperature Non-Equilibrium Plasmas: The LXCat Project, History, Perspectives and a Tutorial

Emile Carbone ^{1,*}, Wouter Graef ², Gerjan Hagelaar ¹, Daan Boer ³, Matthew M. Hopkins ⁴, Jacob C. Stephens ⁵, Benjamin T. Yee ⁴, Sergey Pancheshnyi ⁶, Jan van Dijk ³ and Leanne Pitchford ^{1,†}

E. Carbone et al., *Atoms* (2021), **9** (1), 16.

An introduction to the LXCat website

70 views • Mar 10, 2021

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Youtube tutorial



Contact the LXCat team: info@lxcat.net



*Thank you for your attention and
looking forward to your feedback!*