LXCat 3

A novel data platform for low temperature plasma physics

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Jan van Dijk

2^{nd} Workshop on FAIR Data in Plasma Science

TU/e LXCat

LXCat ("elecscat") [1]

Electron (and ion) collisional processes in plasmas

- **Cross sections**
- Potentials
- Swarm parameters

[1] Carbone, E., Graef, W., Hagelaar, G., Boer, D., Hopkins, M. M., Stephens, J. C., Yee, B. T., Pancheshnyi, S., van Dijk, J., & Pitchford, L. (2021). Data Needs for Modeling Low-Temperature Non-Equilibrium Plasmas: The LXCat Project, History, Perspectives and a Tutorial. *Atoms*, *9*(1), 16. https://doi.org/10.3390/atoms9010016

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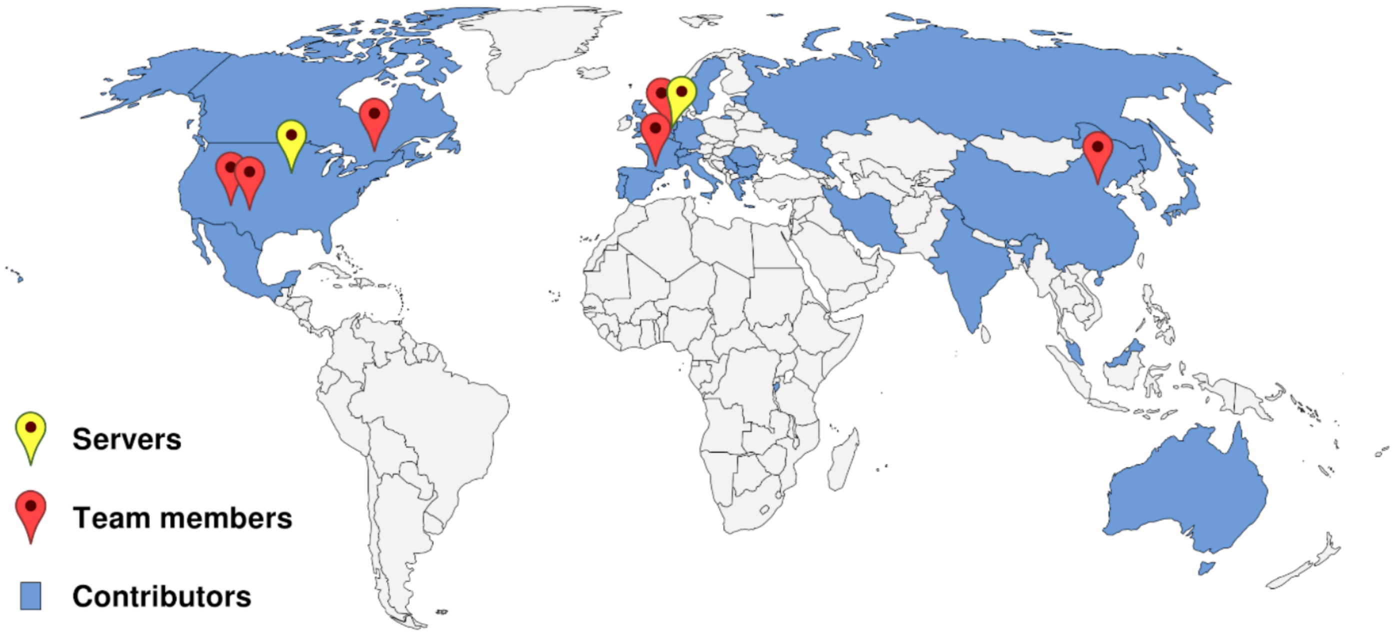
Electron (and ion) collisional processes in plasmas

- **Cross sections**
- Potentials
- Swarm parameters

Statistics

- ≈ 120 visitors/day
- ≈ 30000 cross sections
- International



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Traditionally

- Self-consistent datasets ("mechanisms")
- Combination with two-term Boltzmann solver

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More recently

- State-to-state data
- Request for more detailed annotations
- Request for "chemistries"

An Argon "mechanism"

Complete set

- Elastic (effective)
- Excitation
- Ionization
- (Attachment)

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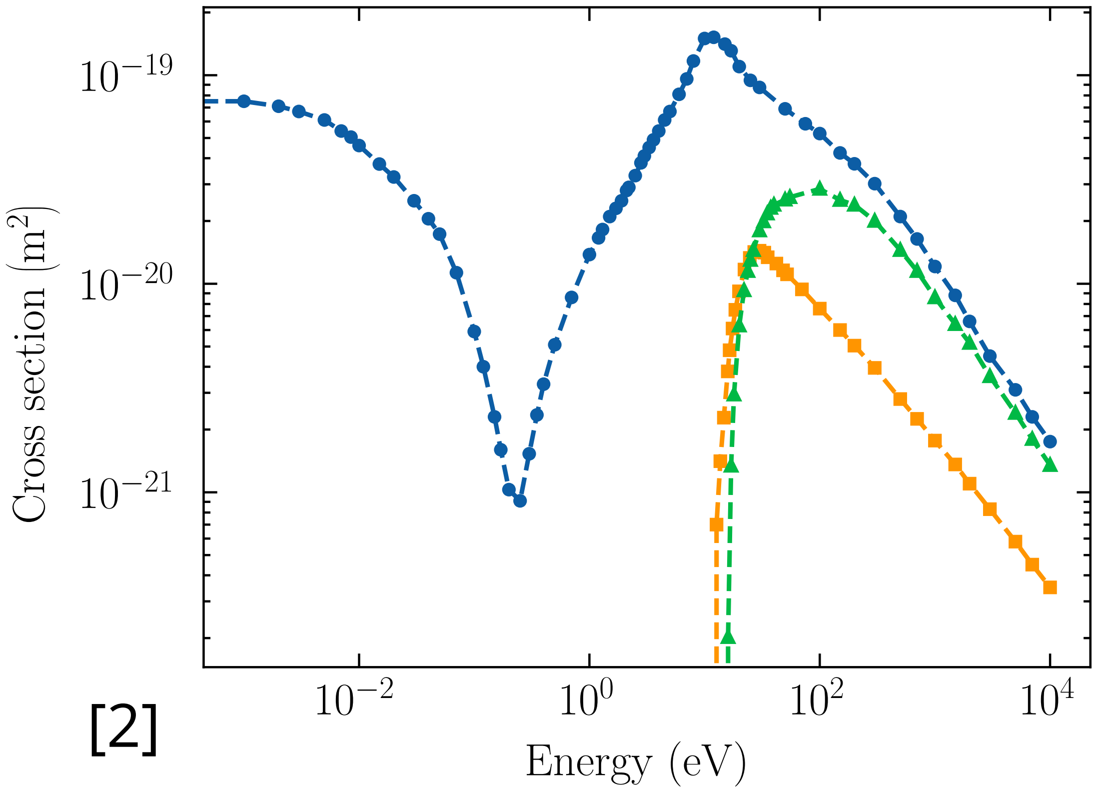
$$e + Ar \rightarrow e + Ar$$

$$e + Ar \rightarrow e + Ar^*$$

$$e + Ar \rightarrow 2e + Ar^+$$



[2]

[2] Yamabe, C., Buckman, S.J. & Phelps, A.V., 1983. Measurement of free-free emission from low-energy-electron collisions with Ar. Physical Review A, 27(3), pp.1345–1352. Available at: http://dx.doi.org/10.1103/PhysRevA.27.1345.

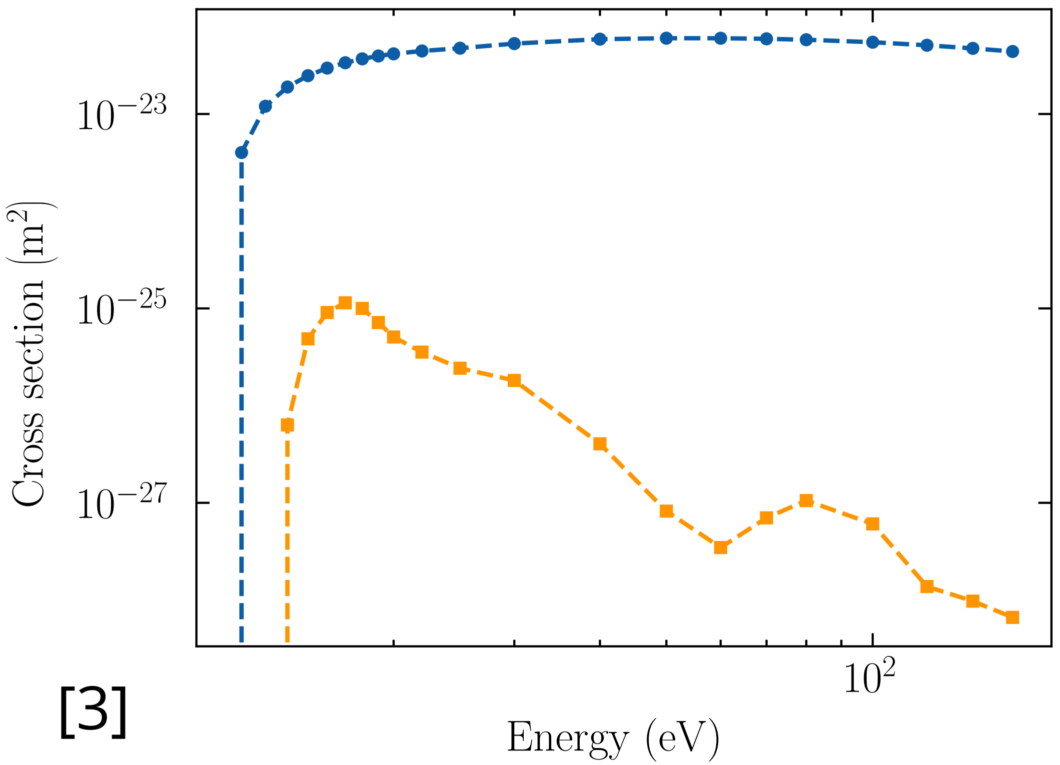
A Hydrogen state-to-state model

Excitation in molecules

- $e + H_2(X^1\Sigma_g^+, \nu = 5) \rightarrow e + H_2(B^1\Sigma_u^+, \nu = 24)$
- $e + H_2(X^1\Sigma_g^+, \nu = 5) \rightarrow e + H_2(j^3\Delta_g, \nu = 8)$
- $\ldots$

A lot more detailed

- Vibrationally resolved
- 341 states
- 4875 reactions



[3]

[3] Scarlett, L.H. et al., 2021. Complete collision data set for electrons scattering on molecular hydrogen and its isotopologues: I. Fully vibrationally-resolved electronic excitation of H2(X1Σg+). Atomic Data and Nuclear Data Tables, 137, p.101361. Available at: http://dx.doi.org/10.1016/j.adt.2020.101361.

Trouble...

Ground states

Ar BCl BCl2 BCl3 BF3 Be C C2 C2H2 C2H4 C2H6 C2OH6 C3 C3H4 C3H6 C3H8 C3N CCl2F2 CCl4 CF CF2 CF3I CF4 CH CH2 CH3 CH4 CHF3 CNH CO CO2 CONH3 COS CS
CaF Cl2 Cu D2 DT F F2 F2O H H2 H2O H2S H4C HBr HCHO HCN HCP HCl HD HT He Hg Kr Mg N N2 N2O NF3 NH3 NO NO2 Na Ne O O2 O3 O- PH3 SF SF2 SF3 SF4
SF5 SF6 SO2 Si2H6 Si(CH3)4 SiF2 SiH4 SiO T2 Xe

State-specific and gas mixtures

Ar* Ar(3d'[3/2]2) Ar(3d'[5/2]2) Ar(3d'[5/2]3) Ar(3d[1/2]0) Ar(3d[1/2]1) Ar(3d[3/2]1) Ar(3d[3/2]2) Ar(3d[5/2]2) Ar(3d[5/2]3) Ar(3d[7/2]3) Ar(3d[7/2]4) Ar(3p5 4p J = 0 2p5)
Ar(3p5 4p J = 1 2p10) Ar(3p5 4p J = 1 2p2) Ar(3p5 4p J = 1 2p4) Ar(3p5 4p J = 1 2p7) Ar(3p5 4p J = 2 2p3) Ar(3p5 4p J = 2 2p6) Ar(3p5 4p J = 2 2p8) Ar(3p5 4p J = 3 2p9)
Ar(3p5 4s J = 0 1s3) Ar(3p5 4s J = 1 1s4) Ar(3p5 4s J = 2 1s5) Ar(3p5 4s j = 1 1s2) Ar(3p6 J = 0) Ar(4p'[1/2]0) Ar(4p'[1/2]1) Ar(4p'[3/2]1) Ar(4p'[3/2]2) Ar(4p[1/2]0) Ar(4p[1/2]1)
Ar(4p[3/2]1) Ar(4p[3/2]2) Ar(4p[5/2]2) Ar(4p[5/2]3) Ar(4s'[1/2]0) Ar(4s'[1/2]1) Ar(4s[3/2]1) Ar(4s[3/2]2) Ar(5s'[1/2]0) Ar(5s'[1/2]1) Ar(5s[3/2]1) Ar(5s[3/2]2) Be(2p(2)1D2)
Be(2p(2)3P2) Be(2s_2p_1P) Be(2s_2p_3P) Be(2s_3d_1D) Be(2s_3d_3D) Be(2s_3p_1P) Be(2s_3p_3P) Be(2s_3s_1S) Be(2s_3s_3S) Be(2s_4d_1D) Be(2s_4d_3D) Be(2s_4f_1F)
Be(2s_4f_3F) Be(2s_4p_1P) Be(2s_4p_3P) Be(2s_4s_1S) Be(2s_4s_3S) BeH+ C2H2+ C(2p(2)_1D) C(2p(2)_1D2) C(2p(2)_1S) C(2p(2)_1S0) C(2p(2)_3P1) C(2p(2)_3P3) C(2p3d_1Do)
C(2p3d_1Fo) C(2p3d_1Po) C(2p3d_3Do) C(2p3d_3Fo) C(2p3d_3Po) C(2p3p_1D) C(2p3p_1P) C(2p3p_1S) C(2p3p_3D) C(2p3p_3P) C(2p3p_3S) C(2p3s_1Po) C(2p3s_3Po) C(2p4s_1Po)
C(2p4s_3Po) C(2p_3d_1D2) C(2p_3d_1F3) C(2p_3d_1P1) C(2p_3d_3D1) C(2p_3d_3D2) C(2p_3d_3D3) C(2p_3d_3F2) C(2p_3d_3F3) C(2p_3d_3F4) C(2p_3d_3P0) C(2p_3d_3P1)
C(2p_3d_3P2) C(2p_3p_1D2) C(2p_3p_1P1) C(2p_3p_1S0) C(2p_3p_3D1) C(2p_3p_3D2) C(2p_3p_3D3) C(2p_3p_3P0) C(2p_3p_3P1) C(2p_3p_3P2) C(2p_3p_3S1) C(2p_3s_1P1)
C(2p_3s_3P0) C(2p_3s_3P1) C(2p_3s_3P2) C(2p_4s_1P1) C(2p_4s_3P0) C(2p_4s_3P1) C(2p_4s_3P2) C(2s2p(3)_3Do) C(2s2p(3)_3Po) C(2s2p(3)_5So) C(2s_2p(3)_3D1) C(2s_2p(3)_3D2)
C(2s_2p(3)_3D3) C(2s_2p(3)_3P0) C(2s_2p(3)_3P1) C(2s_2p(3)_3P2) C(2s_2p(3)_5S2) CH+ CO-rot CO2+ CO2(bend mode) CaF+ Cs* D2(B,v=0) D2(B,v=1) D2(B,v=10) D2(B,v=11)
D2(B,v=12) D2(B,v=13) D2(B,v=14) D2(B,v=15) D2(B,v=16) D2(B,v=17) D2(B,v=18) D2(B,v=19) D2(B,v=2) D2(B,v=20) D2(B,v=21) D2(B,v=22) D2(B,v=23) D2(B,v=24)
D2(B,v=25) D2(B,v=26) D2(B,v=27) D2(B,v=28) D2(B,v=29) D2(B,v=3) D2(B,v=30) D2(B,v=31) D2(B,v=32) D2(B,v=33) D2(B,v=34) D2(B,v=35) D2(B,v=36) D2(B,v=37)
D2(B,v=38) D2(B,v=39) D2(B,v=4) D2(B,v=40) D2(B,v=41) D2(B,v=42) D2(B,v=43) D2(B,v=44) D2(B,v=45) D2(B,v=46) D2(B,v=47) D2(B,v=48) D2(B,v=49) D2(B,v=5)
D2(B,v=6) D2(B,v=7) D2(B,v=8) D2(B,v=9) D2(X,v=0) D2(X,v=1) D2(X,v=10) D2(X,v=11) D2(X,v=12) D2(X,v=13) D2(X,v=14) D2(X,v=15) D2(X,v=16) D2(X,v=17) D2(X,v=18)
D2(X,v=19) D2(X,v=2) D2(X,v=20) D2(X,v=3) D2(X,v=4) D2(X,v=5) D2(X,v=6) D2(X,v=7) D2(X,v=8) D2(X,v=9) D2$^+$(1sSg,v=0) D2$^+$(1sSg,v=1) D2$^+$(1sSg,v=10) D2$^+$(1sSg,v=11)
D2$^+$(1sSg,v=12) D2$^+$(1sSg,v=13) D2$^+$(1sSg,v=2) D2$^+$(1sSg,v=3) D2$^+$(1sSg,v=4) D2$^+$(1sSg,v=5) D2$^+$(1sSg,v=6) D2$^+$(1sSg,v=7) D2$^+$(1sSg,v=8) D2$^+$(1sSg,v=9) D2$^+$(1sSg,v=FC)
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F(2p^4(^3P)5s) H(1S) H2+ H2(+) H(2P) H(2S) H2$^+$(1sSg,v=0) H2$^+$(1sSg,v=1) H2$^+$(1sSg,v=2) H2$^+$(1sSg,v=3) H2$^+$(1sSg,v=4) H2$^+$(1sSg,v=5) H2$^+$(1sSg,v=6) H2$^+$(1sSg,v=7)

Recap: Identify problems

Data format & Semantics

Data storage

Platform design & implementation

Data format & Semantics

Nonstandard format

- Hard to parse
- Duplication

Lack of structured schema

- State notations
- Ambiguity

```
EXCITATION
N2 → N2 (v=0 - v=1)
 3.000000e-1
SPECIES: e / N2
PROCESS: E + N2 → E + N2 (v=0 - v=1), Excitation
PARAM.:  E = 0.3 eV, complete set
COMMENT: [e + N2(X,v=0) ⟷ e + N2(X,v=1), Vibrational]
COMMENT: Pitchford L C and Phelps A V 1982
UPDATED: 2017-09-03 03:54:40
COLUMNS: Energy (eV) | Cross section (m2)
-----------------------------
 3.000000e-1    0.000000e+0
 4.000000e-1    3.000000e-23
 <omitted lines>
-----------------------------
```

$$\mathrm{e} + \mathrm{N_2}\,(\mathrm{X}, \nu = 0) \rightarrow \mathrm{e} + \mathrm{N_2}\,(\mathrm{X}, \nu = 1)$$

Data storage

Relational database

- SQL
- Table-based

Heterogeneous data

- e^-, Ar^*, $Ar\left({}^1S_0\right)$

Particle	Charge	e	S	L	Parity	J
e	-1	NULL	NULL	NULL	NULL	NULL
Ar	0	*	NULL	NULL	NULL	NULL
Ar	0	NULL	0	0	Even	0

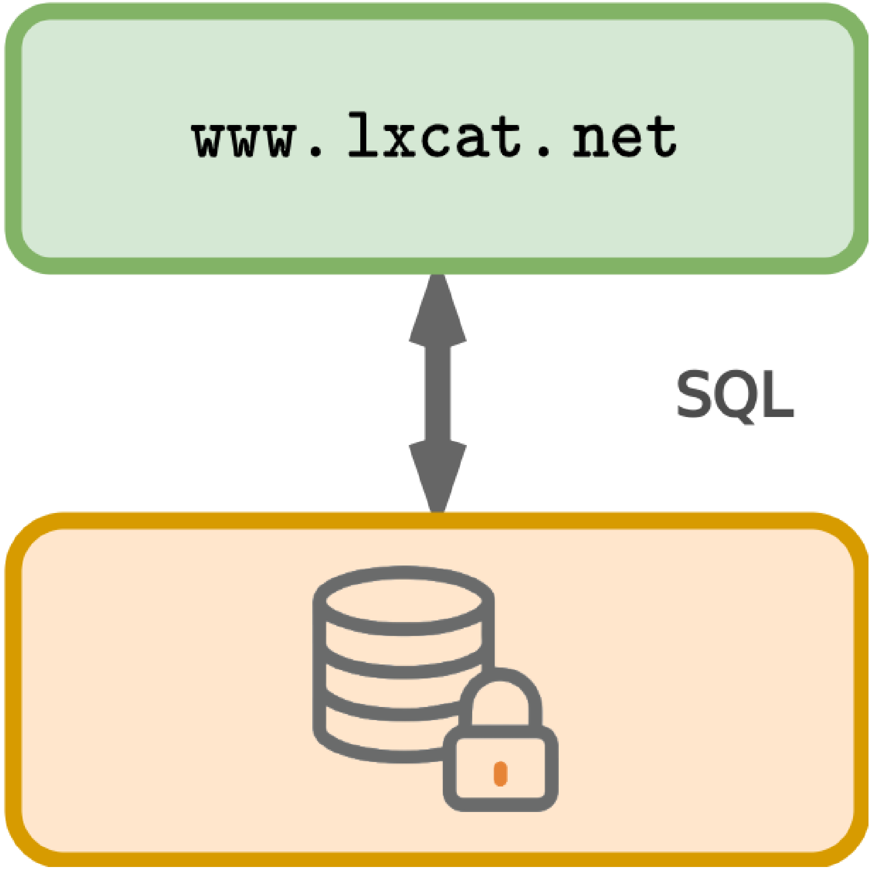
Platform

Intertwined

- Violates separation of concerns

Hard to

- Maintain
- Adapt



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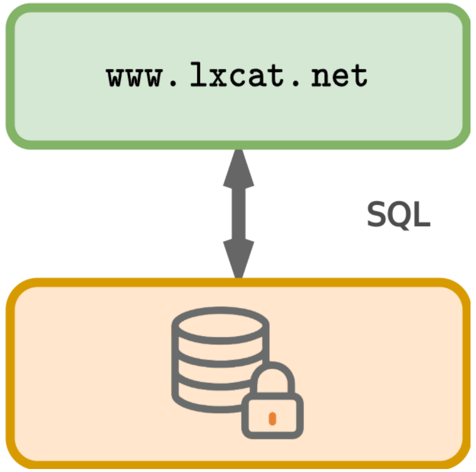
Data storage

Particle	Charge	e	S	L	Parity	J
e	-1	NULL	NULL	NULL	NULL	NULL
Ar	0	*	NULL	NULL	NULL	NULL
Ar	0	NULL	0	0	Even	0

Design & Implementation



A new data format

Universal language

- Captures physics
- Species notation
- Flexible

- JSON
- JSON Schema
- Typescript to JSON Schema generator [4]

[4] https://github.com/vega/ts-json-schema-generator

A new data format

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Examples

He^* →

```
{
  "particle": "He",
  "charge": 0,
  "type": "Unspecified",
  "electronic": "*"
}
```

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}
```

$\mathrm{He}^+\ ({}^2\mathrm{S}_{1/2})$

```json
{
  "particle": "He",
  "charge": 1,
  "type": "AtomLS",
  "electronic": {
    "scheme": "LS",
    "config": [],
    "term": {
      "S": 0.5,
      "L": 0,
      "P": 1,
      "J": 0.5
    }
  }
}
```

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- JSON
- JSON Schema
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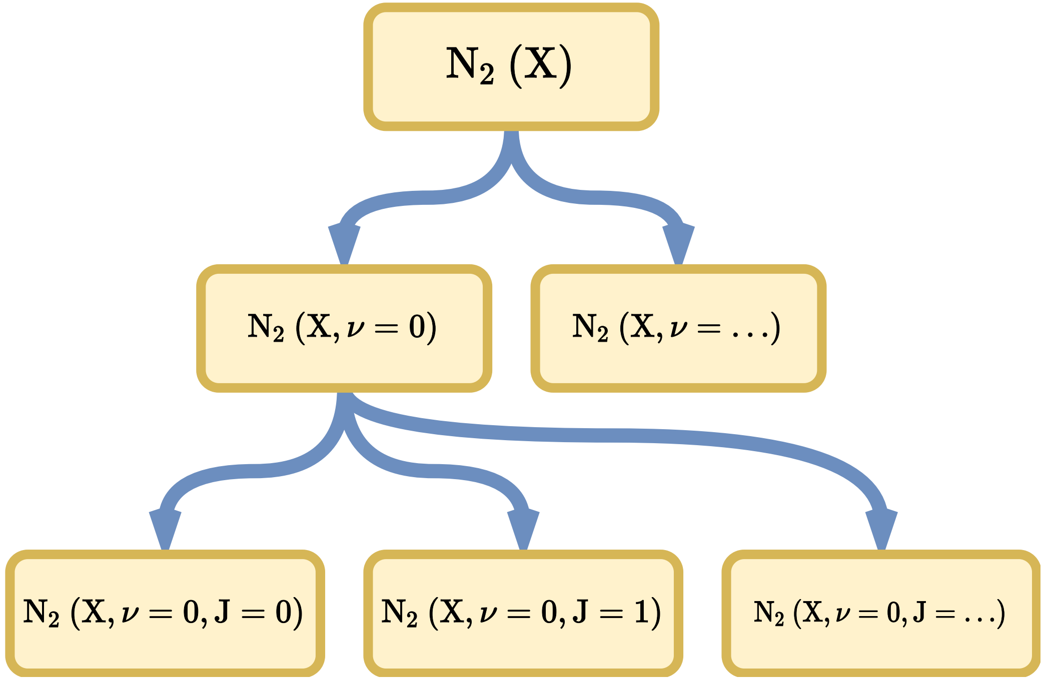
TS **LTP schema generator library**

[4] https://github.com/vega/ts-json-schema-generator

Capturing important relations



- ArangoDB [5]

[5] https://github.com/arangodb/arangodb

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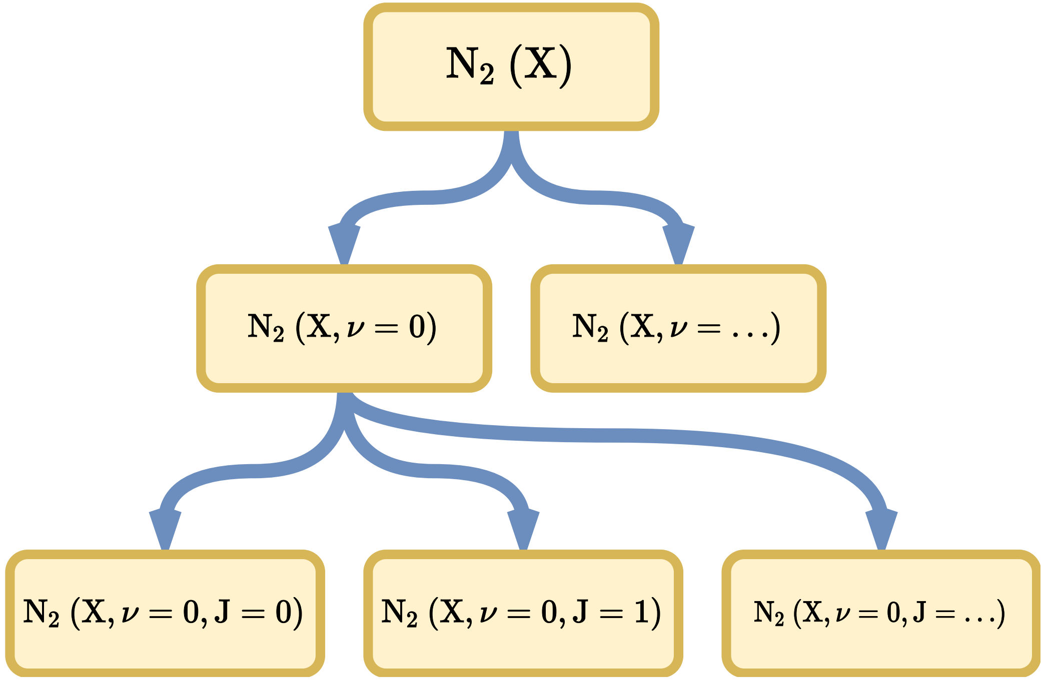

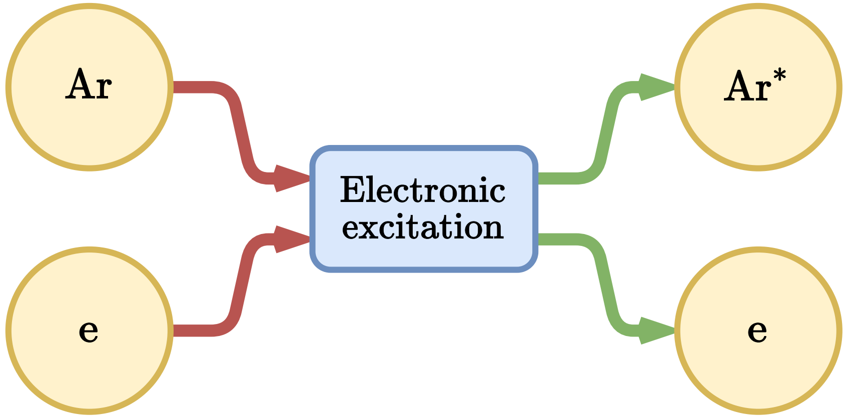

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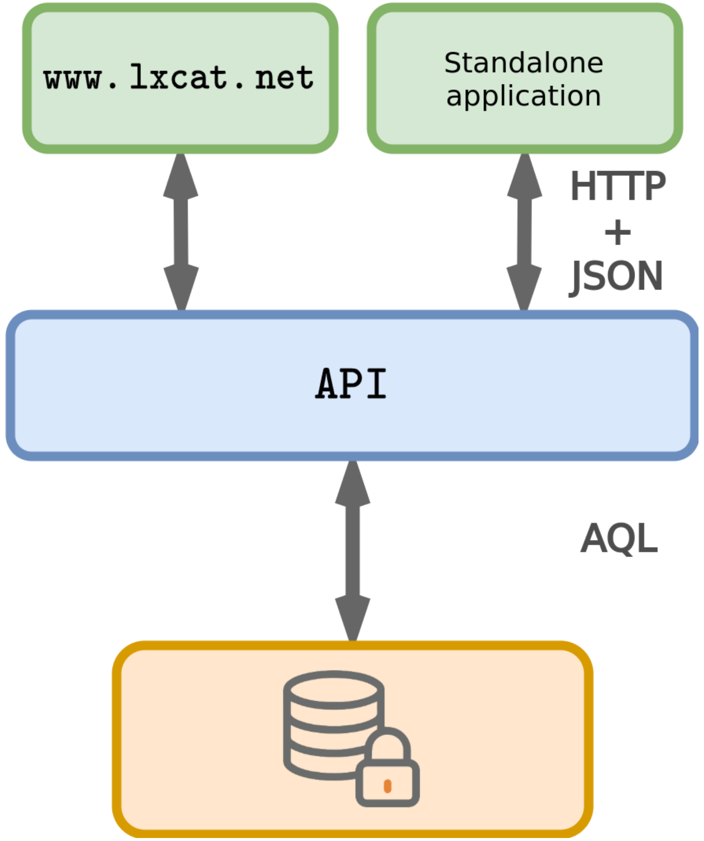
[5] https://github.com/arangodb/arangodb

Web infrastructure



- Next.js + React [6]
- TypeScript
- WebAssembly

[6] https://github.com/vercel/next.js

Outlook

LXCat

- Official release!
- Open-source

https://gitlab.com/LXCat-project/lxcat

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Applications

- LisbOn KInetics Boltzmann solver (LoKI-B) [7]
- Magnum Potential Integrator (MagnumPI) [8]

https://gitlab.com/LXCat-project/lxcat

[7] Tejero-Del-Caz et al. (2019). The LisbOn KInetics Boltzmann solver. *Plasma Sources Science and Technology*, *28*(4). https://doi.org/10.1088/1361-6595/ab0537

[8] https://gitlab.com/magnumpi/magnumpi

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Chemistry

- Collaborations

```
Fetch He-JohnDoe-2023; Run simulation
```

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