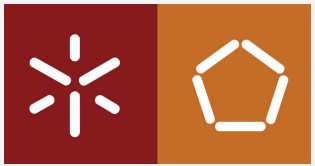
Atomic Data Repository & Interface

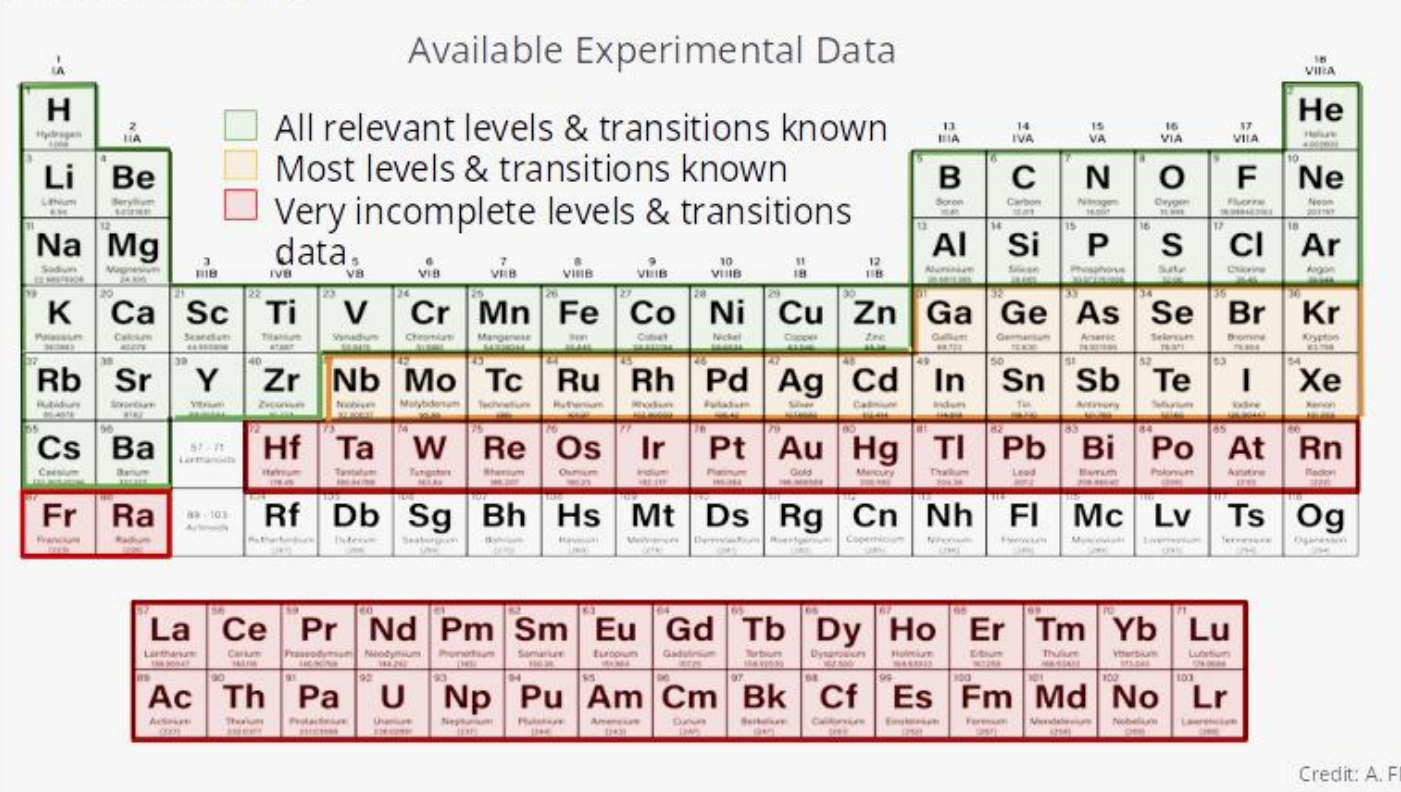
Summer internship

João Freitas, FCUL
Carolina Freitas, UMINHO

Supervisors: Luís Leitão, Ricardo F.Silva, Prof. Dr. José Pires Marques, Tomás Campante



Motivation & Purpose



Motivation & Purpose

- What is the importance of atomic spectra data for lanthanides?
  - Relevance in different scientific fields, such as spectroscopy and astrophysics
  - Necessity for the data only appeared in 2017, with the first recorded kilonova
- Why calculate these levels, transitions and electron-ion collisions?
  - Serves as a short-term solution until experimental data is gathered
  - Easier, faster and cheaper than experimental testing

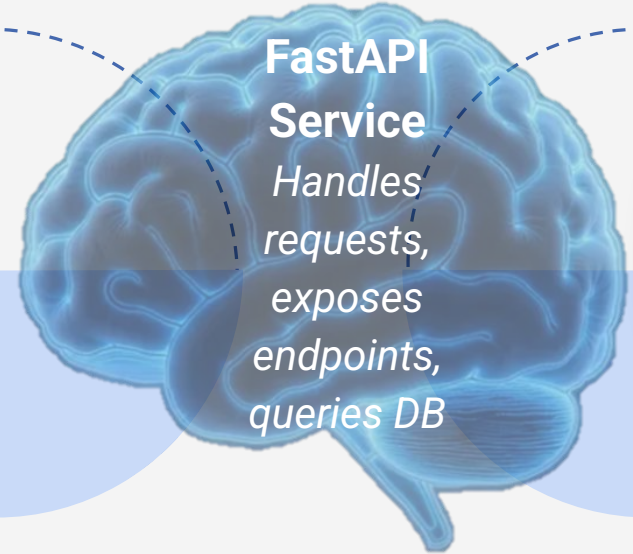
Motivation & Purpose

- Purpose of the system:
  - Reliable relational repository for calculated atomic data
  - Scientific provenance & traceability
  - Availability for the wider scientific community
  - User friendly web interface
  - Providing previously unavailable data

High-Level Architecture

User Interface

Sends HTTP requests via REST API



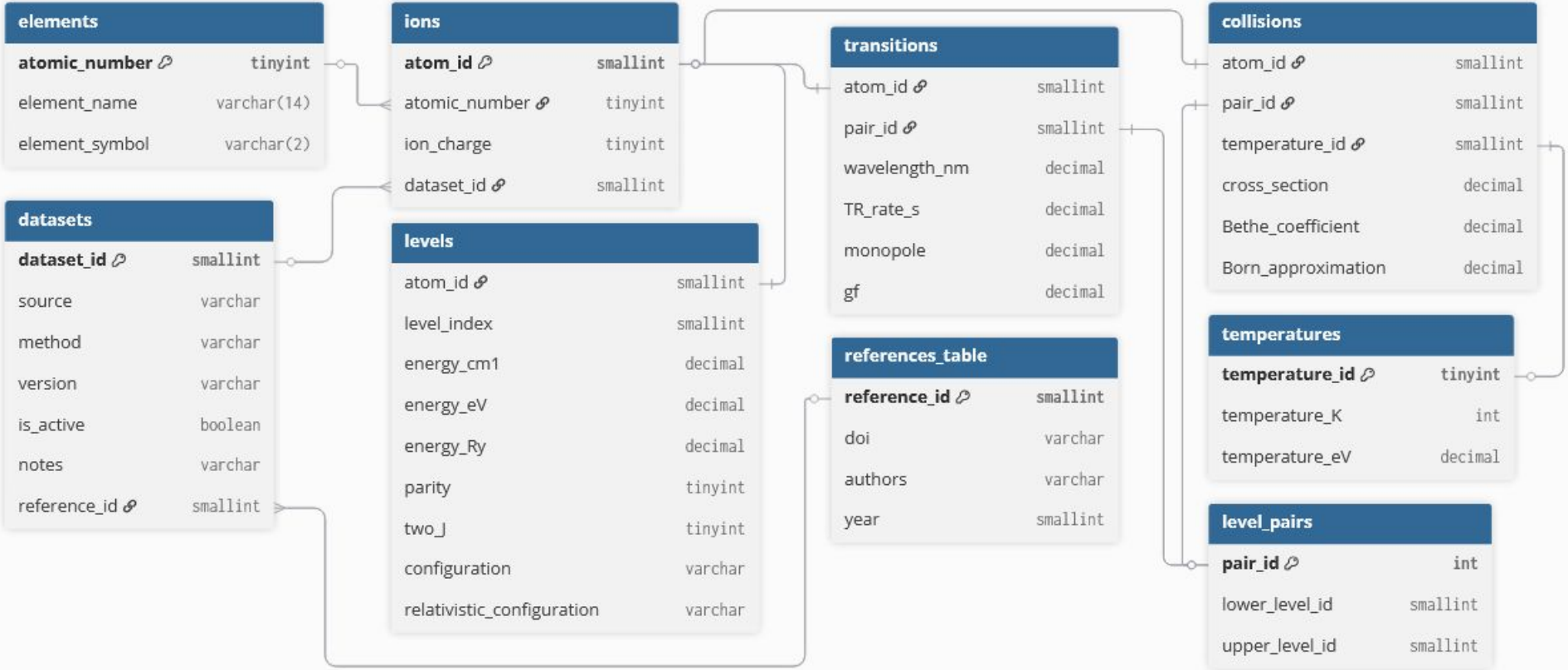
FastAPI Service

Handles requests, exposes endpoints, queries DB

MySQL (DataBase)

Formatted data storage, referential integrity in a relational schema. It's read from and written to by the API

Database Schema



Tools used

Database and data processing

- MySQL 8.0 for the DataBase Management System (DBMS)
- Python for reading and parsing the raw data
  - Also used for formatting the data for ingestion
- MySQL-connector-python and SQLAlchemy python packages for querying the database and ingesting new data

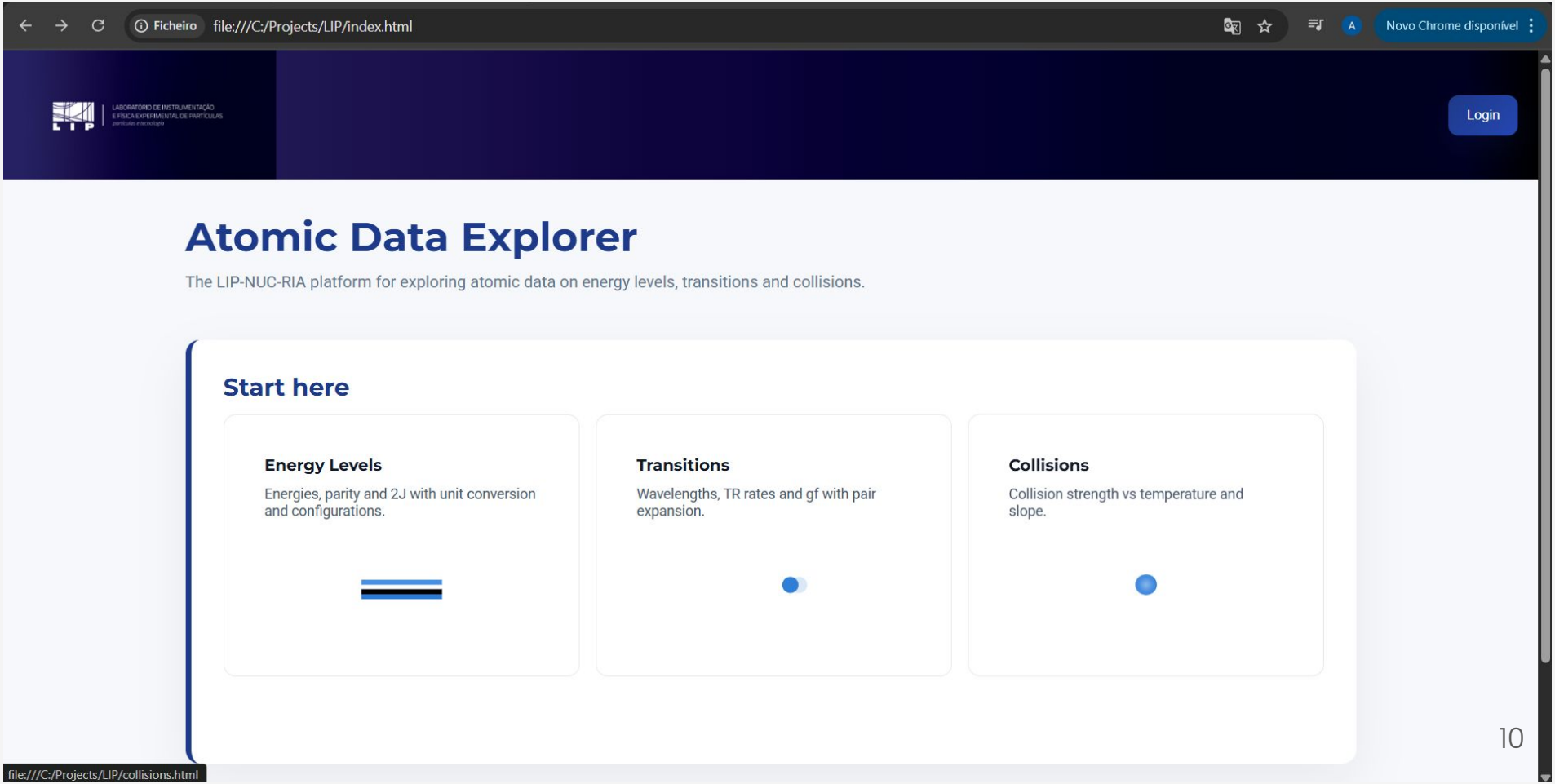
Tools used
Website and API

- HTML5, CSS3 and JavaScript ES6+ for the frontend
- Uvicorn as a server
- Browser DevTools, Postman and Insomnia for running tests
- FastAPI (builds in Python Restfull API) to strengthen API

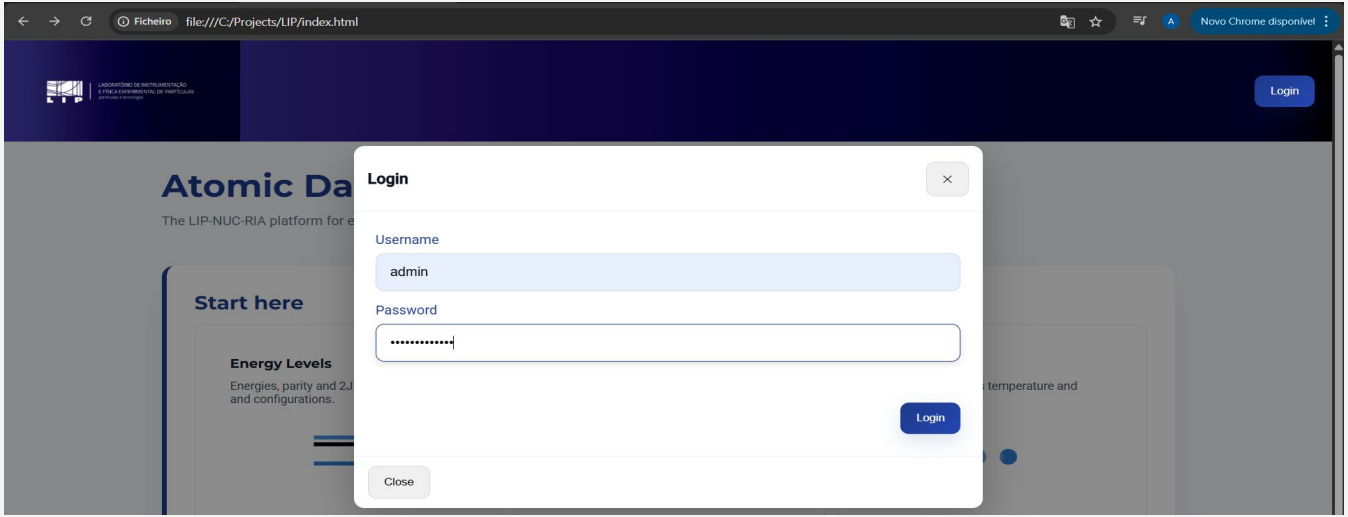
Some precautions taken

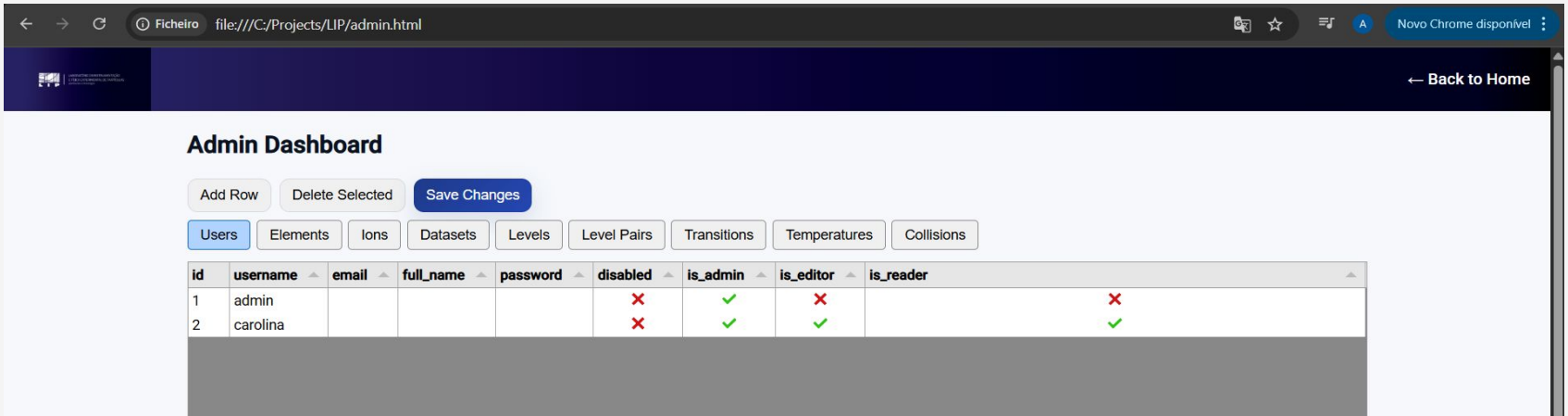
- **Security:** Communication is secured through digital certificates for encryption.
- **CORS (Cross-Origin Resource Sharing):** Manages the permissions of the frontend communication only with the API.
- **Separation of modules:** UI code is completely separate from API code and from the database server itself, promoting modularity and maintainability of each module.
- **SQL injection prevention:** Code is written so that queries cannot alter the database, only access it.

User Interface - Main page



User Interface - Administration





User Interface – Levels

Ficheiro file:///C:/Projects/LIP/levels.html

Novo Chrome disponível

← Back to Home Admin Dashboard

Energy Levels

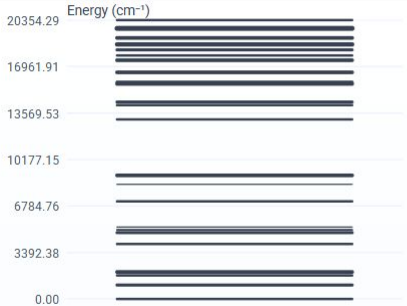
La	II	Energy unit: cm⁻¹	Level range: 1	25	Configurations	Relativistic configurations

Methods | Details | Show Diagram

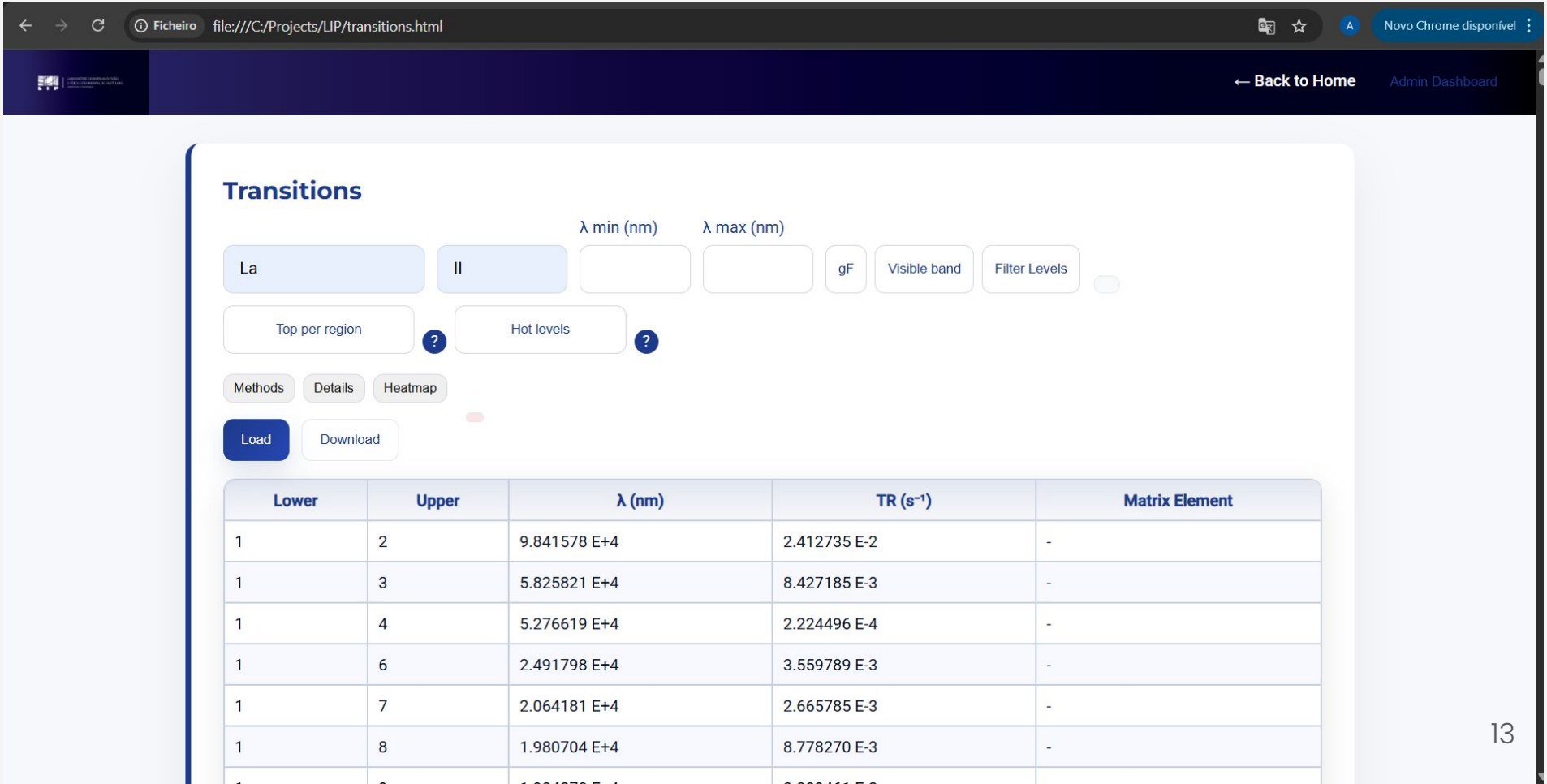
Load | Download

Index	Energy ↑	Parity	2J
1	0	0	4
2	1.016097 E+3	0	6
3	1.716496 E+3	0	4
4	1.895153 E+3	0	2
5	1.970703 E+3	0	8
6	4.013166 E+3	0	4
7	4.844537 E+3	0	6

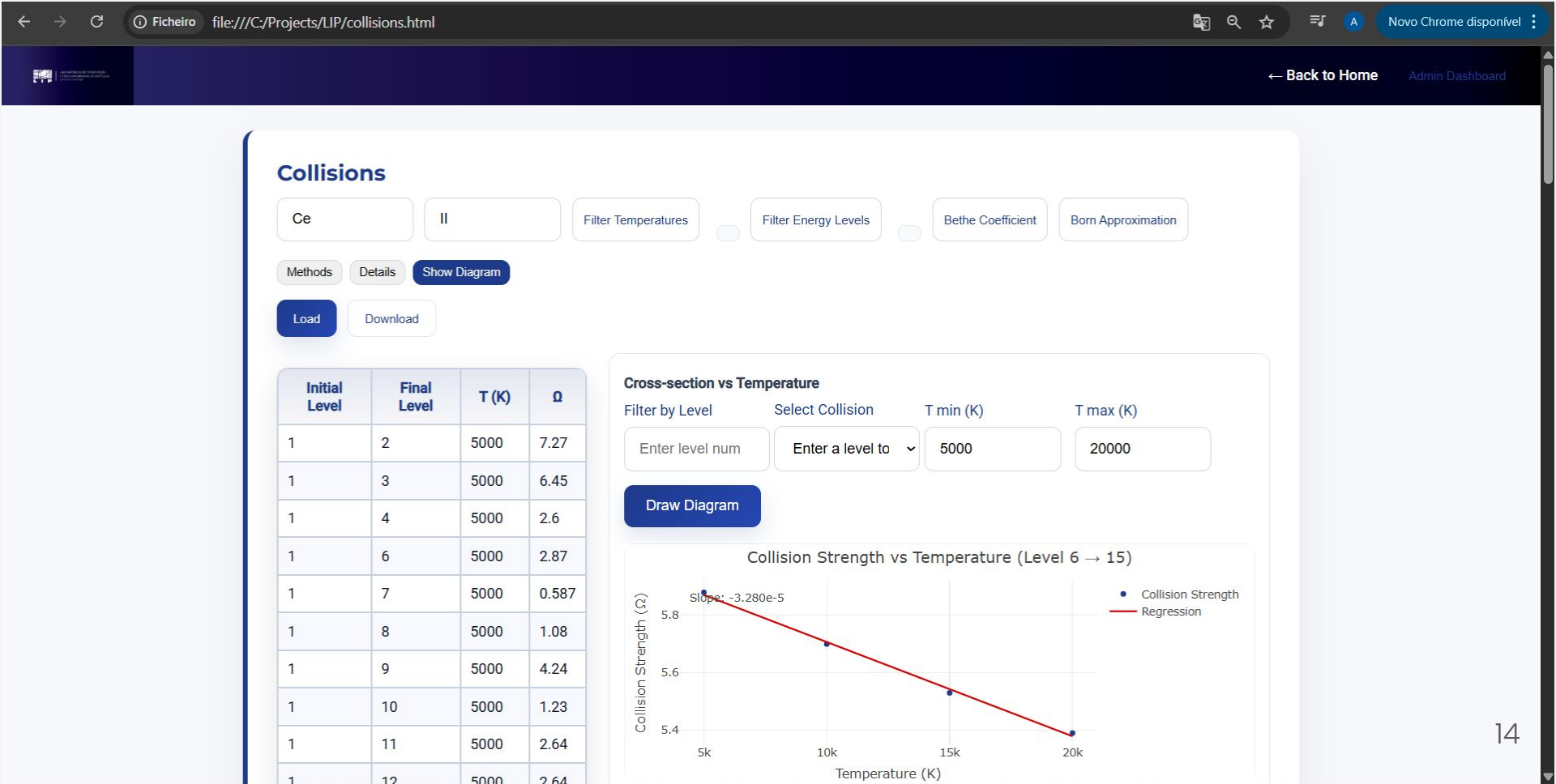
Energy level diagram



User Interface - Transitions



User Interface - Collisions



Database - Levels example

Local instance MySQL80

File Edit View Query Database Server Tools Scripting Help

fetch-all | SQL File 5* | SQL File 6* | SQL File 7* | SQL File 7* | Administration - Data Export

Limit to 50000 rows

```
1  select * from elements;
2  select * from references_table;
3  select * from datasets;
4  select * from ions;
5  select * from levels;
6  select * from pairs;
7  select * from transitions;
8  select * from temperatures;
9  select * from collisions;
10
```

Result Grid | Filter Rows: | Export: | Wrap Cell Content:

level_index	atom_id	energy_cm	energy_eV	energy_Ry	parity	two_J	configuration	relativistic_configuration
1	1	0.0000000000	0.0000000000	0.0000000000	0	8	4f2	4f-2(8)8
1	2	0.0000000000	0.0000000000	0.0000000000	0	4	5d2	5d-2(4)4
1	3	0.0000000000	0.0000000000	0.0000000000	0	3	5d1	5d-1(3)3
1	4	0.0000000000	0.0000000000	0.0000000000	1	7	4f1 5d2	4f-1(5)5.5d-2(4)7
1	5	0.0000000000	0.0000000000	0.0000000000	1	8	4f3 6s1	4f-3(9)9.6s+1(1)8
1	6	0.0000000000	0.0000000000	0.0000000000	1	9	4f3	4f-3(9)9
2	1	1528.3199342043	0.1894875220	0.0139270760	0	10	4f2	4f-1(5)5.4f+1(7)10
2	2	1016.0972251833	0.1259800000	0.0092593592	0	6	5d2	5d-1(3)3.5d+1(5)6
2	3	1603.2299317440	0.1987751780	0.0146097061	0	5	5d1	5d+1(5)5
2	4	987.5882212576	0.1224453340	0.0089995661	1	9	4f1 5d2	4f-1(5)5.5d-1(3)8.5d+...
2	5	441.9499806433	0.0547948141	0.0040273446	1	10	4f3 6s1	4f-3(9)9.6s+1(1)10
2	6	1398.3399351160	0.1733720560	0.0127426111	1	11	4f3	4f-2(8)8.4f+1(7)11
3	1	3127.0998633919	0.3877109700	0.0284962307	0	12	4f2	4f+2(12)12
3	2	1716.4958896391	0.2128183670	0.0156418615	0	4	5d2	5d-1(3)3.5d+1(5)4
3	3	7195.1396809813	0.8920836260	0.0655669372	1	5	4f1	4f-1(5)5
3	4	1410.2714636385	0.1748513770	0.0128513392	1	9	4f1 5d2	4f-1(5)5.5d-2(4)9
3	5	1649.0099268682	0.2044511740	0.0150268841	1	12	4f3 6s1	4f-2(8)8.4f+1(7)11.6s...
3	6	2893.1398719953	0.3587036280	0.0263642304	1	13	4f3	4f-1(5)5.4f+2(12)13
4	1	3276.6598575970	0.4062540460	0.0298591216	1	8	4f1 5d1	4f-1(5)5.5d-1(3)8
4	2	1895.1527933330	0.2349690000	0.0172699030	0	2	5d1 6s1	5d-1(3)3.6s+1(1)2
4	3	8695.4096052343	1.0780933900	0.0792384026	1	7	4f1	4f+1(7)7
4	4	1873.8907693557	0.2323328450	0.0170761491	1	7	4f1 5d2	4f+1(7)7.5d-2(4)7
4	5	1743.7199233668	0.2161937170	0.0158899451	1	10	4f3 6s1	4f-2(8)8.4f+1(7)11.6s...
4	6	4453.7598012831	0.5521958390	0.0405856456	1	15	4f3	4f+3(15)15
5	1	3762.7498332471	0.4665215220	0.0342886994	0	4	4f2	4f-2(4)4
5	2	1970.7027433908	0.2443360000	0.0179583648	0	8	5d2	5d+2(8)8
5	3	13591.1394453619	1.6850865300	0.1238515756	0	1	6s1	6s+1(1)1
5	4	2140.4426236743	0.2653810630	0.0195051484	1	1	4f1 5d2	4f-1(5)5.5d-2(4)1
5	5	2998.3598690941	0.3717492450	0.0273230655	1	14	4f3 6s1	4f-1(5)5.4f+2(12)13.6...
5	6	9370.6596052694	1.1618137200	0.0853917334	1	3	4f3	4f-2(8)8.4f+1(7)3
6	1	3821.5298317613	0.4738093130	0.0348243422	1	4	4f1 5d1	4f-1(5)5.5d-1(3)4

elements 1 | references_table 2 | datasets 3 | ions 4 | levels 5 | pairs 6 | transitions 7 | temperatures 8 | collisions 9

Result Grid | Form Editor | Field Types | Query Stats | Execution Plan

Read Only

Query Completed

Future work

- Expanding the database to have data from outside sources
- Integrating calculation of Bethe coefficient and Born approximations for electron-ion collisions
  - Already implemented in the database but no data is available
- Creating python scripts for data from other methods
- Publishing the website and deploying the database
- Machine learning engine searching patterns in data
- More graphical visualization of the phenomena


Questions?!