Contribution ID: 23

Atomic, Molecular and Plasma-Material Interaction Databases at the IAEA

Tuesday, 12 November 2024 11:05 (40 minutes)

The Atomic and Molecular Data (AMD) Unit [1] operates within the Nuclear Data Section (NDS) of the International Atomic Energy Agency with the primary objective to establish and maintain internationally recommended numerical databases of fundamental atomic and molecular data for fusion energy research and other plasma science and technology applications.

The CollisionDB database [2] is an important resource for plasma modellers which contains 122,612 collision cross section and rate coefficient data sets. This FAIR-compliant service is based on a relational database backend with complete metadata and an online, browser-based search interface which allows for data visualization. All data are timestamped, can be deprecated (but not deleted) and are associated with full bibliographic information concerning their source.

The CollisionDB service also exposes an API and a Python library, PyCollisionDB [3], has been released to utilise the API in that language.

A new database of plasma-material interaction data is under development. pwiDB [4] contains data sets concerning the sputtering, retention, diffusion, solubility and permeation of fuel and other ions in fusion reactor materials. In addition to online searching and visualization, data and all necessary contextual metadata can be downloaded in JSON format.

The AMD Unit's databases adopt common standards for the description of units [5], atomic and molecular species, states [6] and processes [7], agreed through experts' meetings and consultancies.

[1] https://amdis.iaea.org/

[2] https://amdis.iaea.org/db/collisiondb/

[3] https://github.com/IAEA-NDS/pycollisiondb

[4] https://db-amdis.org/pwidb/

[5] https://github.com/xnx/pyqn

[6] https://github.com/xnx/pyvalem

[7] https://amdis.iaea.org/databases/processes/

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Session Classification: Web Interfaces and APIs Developments