2023 Helmholtz – OCPC – Programme

for the involvement of postdocs in bilateral collaboration projects

PART A

Title of the project:

Improving the EIRENE-related atomic and molecular data processing

Helmholtz Centre and/or institute:

Forschungszentrum Jülich GmbH

Project leader:

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https://www.fz-juelich.de/de/iek/iek-4
www.eirene.de

Department: (at the Helmholtz centre or Institute)

Institute of Energy and Climate Research, Plasmaphysics (IEK-4)

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Description of the project (max. 1 page)**:**

Providing import of various atomic and molecular data including alternative sources is a very essential part of EIRENE development [www.eirene.de]. In fact, the existing CRMs as well as the underlying datasets (PLOUTOS unifying earlier developed: AMJuel, H2Vibr, HydHel and HydKin) are established as a real highlight with an own value. However, the recent availability of the massive high quality RMPS and CCC calculated data for high-Z atomic as well as molecular species with resolution by isotopes and rovibrational states leads to dramatic increase of the data amounts. Many typical stages of the data processing involving human effort become unrealistic by such data amounts. So, one needs to provide the following:

1) Develop data formats and conversion routines for all significant data types currently available including full support for the older EIRENE-related data.

2) Provide flexibility for assembling the data including the alternative sources, scarce data, variable resolution and accuracy by master files in mark-up formats (JSON, XML or similar)

3) Develop physics-based scalings for isotopes or isotopomers allowing covering of the data gaps.

4) Develop a set of automatic checks (and general data implementation/update polices) to insure the consistency and general quality of the data. Some of the checks have to be based on data visualisation and manipulation tools provided by the toolkit PLOUTUS.

5) Leas with partners (data producers, codes working in coupling to EIRENE, close related PSI codes like ERO, alternative CRM developers e.g. YACORA etc.) on the unification of the basic data formats, datasets and master files.

6) Assist in development of EIRENE access layer to this data together with colleagues working on general EIRENE CRM development (F.Cianfrani, D.Borodin).

7) Validate the implementation of charge-exchange reactions between neutrals and bulk ions in EIRENE. Investigate the scaling with internal vibrational quantum number for molecules and compare with existing data in H2VIBR.

8) Provide EIRENE output for the charge exchange neutrons (CXN) useful for the erosion and other plasma-wall interaction studies.

9) Validate the datasets with diagnostic data (directly as well as through EIRENE applications). Compare the data with alternative databased and literature. Identify and quantify main uncertainties.

10) Provide detailed data documentation including the easily trackable source, uncertainty, history of use in application etc. for every rate or cross-section.

Description of existing or sought Chinese collaboration partner institute (max. half page)**:**

ASIPP Hefei

Through long previous contact and collaboration as well as communication within the ITPA (ITER, International Tokamak Physics Activity (ITPA) (iter.org)) it is very expectable to have a lot of interest in such modelling and development in a view of applications for EAST and other upcoming devices like CFETR.

Required qualification of the postdoc:
- PhD in Physics, Computer Science
- Experience with A&M databases, EIRENE simulations
- Additional skills in Collisional Radiative Models, Fortran programming,
- Language requirement: English.