

## 2 STUDENT ASSISTANT (RESEARCH HIWI) POSITIONS

### MOLECULAR NETWORK ANALYSIS IN ASTROCHEMISTRY

#### Contact:

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**Description:** Astrochemistry is the study of the abundance and reactions of molecules in the Universe [1]. Molecular Network Analysis represents an excellent tool to analyze complex (astro)chemical systems as complete as possible [2], covering a wide range of applications, including Astrochemistry [3], Prebiotic Chemistry [4] or Biochemistry [5]. Molecular networks are represented by molecules (detections) as nodes and transformations/reactions as edges. A current key problem in Astrochemistry is that transformations/reactions are unknown for many samples, e.g. protostellar or cometary systems.

Interested students can choose between several projects about molecular Network Analysis in Astrochemistry, e.g.

- *Surface alteration on simulated moons and comets* – Various types of irradiation (e.g. ions, electrons or photons) modify the surface of planetary bodies and comets. However, the detailed mechanisms are unknown and will be addressed by molecular Network Analysis. More information can be found here: [6].
- *Connection between organic and metalorganic compounds in meteorites* – Recently, previously unknown organomagnesium compounds got detected in meteorites that might present key species in preserving life-relevant organic molecules on early Earth. However, their detailed connection to organic compounds remains unknown and will be addressed by means of Network Analysis. More information can be found here: [7].

Technically, Network Analysis will be performed using the previously developed method mol2net in Python ([github.com/rufalexan/mol2net](https://github.com/rufalexan/mol2net)). Regular meetings (learning skills about how to present results) with the research supervisors will be part of the project. The project aims to result in peer-reviewed publications.

If you are interested in a guided research project, please send your CV and transcript of records to Dr. Alexander Ruf or Prof. Dr. Lukas Heinrich via email and we will arrange a meeting to talk about potential topics. There are currently two vacant project positions.

**Prerequisites/Desired background:** Basic knowledge of UNIX-based operating systems and some experience with programming languages (preferably Python) is helpful, but not required. Students from Chemistry, Physics, Computer Science or any related field are welcome to apply.

**Salary:** 450 Euro / month basis

**Start:** 01/11/2022

#### References

- (1) Ruf, A. u. a. Data-Driven Astrochemistry: One Step Further within the Origin of Life Puzzle. *Life* **2018**, *8*, 18.
- (2) Jeong, H. u. a. The large-scale organization of metabolic networks. *Nature* **2000**, *407*, 651–654.
- (3) Jolley, C. C. u. a. A network-theoretical approach to understanding interstellar chemistry. *The Astrophysical Journal* **2010**, *722*, 1921.
- (4) Wołos, A. u. a. Synthetic connectivity, emergence, and self-regeneration in the network of prebiotic chemistry. *Science* **2020**, 369.
- (5) Kim, H. u. a. Universal scaling across biochemical networks on Earth. *Science advances* **2019**, *5*, eaau0149.
- (6) Ruf, A. u. a. Previously unknown class of metalorganic compounds revealed in meteorites. *PNAS* **2017**, *114*, 2819–2824.
- (7) Ruf, A. u. a. Sulfur ion irradiation experiments simulating space weathering of Solar System body surfaces-Organosulfur compound formation. *Astronomy & Astrophysics* **2021**, *655*, A74.