Disequilibrium chemistry of exoplanets' high-metallicity atmospheres in JWST times

Keywords

Exoplanet atmospheres, chemical kinetics, photochemistry, numerical methods.

Project description

The observations made in the first two years of operation of the James Webb Space Telescope (JWST) are offering unprecedented insights into the composition, dynamics and energetics of a broad range of exoplanet atmospheres. Given the complexity of atmospheric phenomena, the data will be scrutinized with the aid of sophisticated models for many years to come. The ARIEL space mission, to be launched in 2029 to survey ~1,000 warm and hot exoplanets, will contribute in due course to the ongoing revolution of our understanding of exoplanet atmospheres.

The term *disequilibrium* has emerged as a keyword in the cutting-edge investigation of exoplanet atmospheres. Indeed, a main finding of the first JWST spectrum of an exoplanet[1] is the occurrence of atmospheric SO_2 in abundances unexplained by equilibrium chemistry. Modeling atmospheres in disequilibrium is complex yet essential for the correct interpretation of the spectra obtained by JWST and future telescopes. The modeling becomes ever more challenging for high-metallicity atmospheres (i.e. rich in elements other than H and He), because the possibilities for neutral and ion chemistry are significantly more diverse. Given that the field is steadily shifting towards the characterization of low-mass planets with possibly secondary atmospheres, and with the ultimate goal of characterizing the first Earth-twin planet in a not-too-distant future, this is the time to invest in the modelling of their atmospheric chemistry.

The present project is concerned with the modelling of disequilibrium chemistry in exoplanet atmospheres of high metallicity. Its goal is twofold.

The first goal is to investigate the implications of disequilibrium chemistry in the atmospheres of JWST targets for which transmission spectra exist or will be available soon. The list of such targets and published spectra is rapidly expanding. The proposed work will benefit from an in-house photochemical model [GM07] that includes the relevant processes for neutral-ion photochemistry. The PhD candidate will tune the chemical network to the needs of the problem, exploring possible deficiencies in our knowledge of the chemical kinetics. The work will emphasize the significance of metal-catalyzed reactions involving either neutrals or ions and their implications on observables such as SO_2. We will use the software PUMPKIN [MA14] to identify the chemical pathways that control the simulated compositions. We will turn this knowledge into recommendations about chemical reactions that should be better quantified in laboratory experiments or through computational chemistry calculations.

The second goal of the project is concerned with exploring the effect of super-thermal chemistry in exoplanet atmospheres. Super-thermal chemistry is driven by particles that have high kinetic energies and are produced by exothermic reactions. This type of disequilibrium chemistry has never been explored in the atmospheres of exoplanets, yet there is evidence that it plays a major role in the atmospheres of the Solar System planets and their laboratory analogs [HO12] and that may have acted as an intermediate step in the creation of amino acids in early Earth [SA71]. In recent years, Dr. García Muñoz has developed the numerical tools for the simulation of non-thermal particles

[1] https://www.jwst.fr/2022/12/wasp-39b-webb-revele-latmosphere-dune-exoplanete-comme-jamais-auparavant/

[GM23a,b] that will enable the student and collaborators to explore these ideas. Given that most of the tools are in place, the potential for rapid and impactful progress is high.

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Timeliness, skills acquired & team

The PhD topic is timely as there is a clear need for the interpretation of the exoplanet spectra being measured by JWST and, further into the future, by ARIEL. The project will help train the PhD candidate in the complex physics and chemistry of planetary atmospheres, and the relevant numerical methods. There will be many opportunities for interacting with other groups at the (inter-)national level through e.g. the ARIEL Consortium.

The PhD candidate will be supervised by Dr. García Muñoz, at CEA Paris-Saclay. The project takes place at the Laboratoire Dynamique des Etoiles, des Exoplanètes et de leur Environment (LDE3/DAp), which is composed of experts in astrophysical fluid dynamics and exoplanets involved in the JWST, ARIEL and PLATO missions. To go beyond:

http://irfu.cea.fr/dap/LDEE/index.php (http://irfu.cea.fr/dap/LDEE/index.php)
https://antoniogarciamunoz.wordpress.com/

Candidate profile

The candidate must have a Masters in Astrophysics or a related field (e.g. Applied Mathematics or Engineering) and a strong interest in theoretical/numerical work and in the comparison of observations with model simulations. In particular, the candidate must:

- be proficient in scientific programming (one of fortran, C, C++).
- be proficient in numerical simulations of physical systems.
- have some knowledge of or the interest to learn about chemical kinetics.
- be willing to learn about exoplanet atmospheres.