

Proposition de Projet de Recherche Doctoral, Initiative Physique des Infinis The H₂ molecule as a tracer of turbulence and mixing: interpreting JWST data

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Scientific context: How galaxies form is one of the main question of contemporary astrophysics. In the current dark matter-dominated cosmological model, galaxies are assembled from the collapse of gas in virialized dark matter halos. However, predicting the physical properties of galaxies (like their star formation rates or morphologies) is still very challenging, essentially because we still do not fully understand which processes regulate the gas content in galaxies. Those processes involve a complex interplay between gravitational collapse, gas accretion via cold gas streams infalling from the cosmic web, galaxy merging, and feedback related to star formation and/or active galactic nuclei (AGN, i.e. galaxies hosting an active supermassive black hole). It is this balance between the rates of inflow, outflow, and star formation that gives the physical characteristics of the galaxies we observe today.

To grow a galaxy, baryons must cool down to form new stars, but the energy liberated by accretion and feedback from stars and black holes limits the gas cooling. *The impact of this injection of energy on the build-up of galaxies is largely unknown, and depends on how that energy is transferred to the gas.* Some of this energy is thermalized, producing halos of hot gas with long cooling timescales. Some of it is transferred as bulk kinetic energy by radiation pressure or direct mechanical impact, producing galactic winds. **Part of the kinetic energy injected on large scales by feedback is transferred to smaller scales where stars are forming, which sustains turbulence in the molecular gas and mixing across gas phases.** This third point is largely ignored in current studies of galaxy formation, and only captured in cosmological simulations over a very limited range of scales. Because it has a strong impact on the gas cooling, the dissipation of turbulence may be a key process in regulating the gas content of galaxies, but **little is known about the impact of mixing on the formation and excitation of the molecular gas.**

The James Webb Telescope (JWST) is opening a fully new perspective, with high spatial resolution spectro-imaging of the H₂ molecule, which is the most efficient molecular coolant of gas heated by mechanical energy. Spitzer observations have revealed that a large fraction of the mechanical energy injected by feedback is stored in a turbulent reservoir, and cascades down to small scales, where it is dissipated, in particular through H₂ lines (e.g. Guillard+2009, Ogle+2012, Lesaffre+13, Emonts+2016). The rotational lines of H₂ integrated over entire galaxies radiate, in many sources, a total power that cannot be explained by the sole reprocessing of the available UV radiative energy (e.g. Guillard et al. 2009, 2012). Recently, JWST and ALMA observations of the Stephan's Quintet galaxy collision have revealed a complex pc-scale structure of the molecular gas in the intergalactic medium, which suggests that the warm (>100K) H₂ gas may be formed out of cold (20K), CO-emitting, molecular clumps being shattered, mixed and entrained with the hot, X-ray emitting gas.

We would like to investigate, **with numerical simulations**, the impact of cloud shattering and mixing on the formation and excitation of warm H₂ gas, which radiates strongly in the infrared. This is crucial to interpret JWST data, and we would like to involve a PhD student in our project.

Science objectives: In astrophysical environments where large amounts of mechanical energy are involved, like AGN or galaxy interactions, H₂ lines can be unambiguous tracers of turbulent dissipation. **However, we still miss a comprehensive model of the mass and energy transfer rates between gas phases, to provide a quantitative interpretation of the H₂ line emission, the formation of molecular gas within hot gas, and the observed cooling flow across gas phases.** *The objective of this PhD project is, thanks to numerical simulations, to develop a physical framework where multi-wavelength observations, including H₂ line fluxes that will be measured by JWST in thousands of galaxies, are combined to quantify the cooling rates from hot-to-warm and warm-to-cold phases.*

Observationnally, the mass and energetics of the gas within each phase (ionized, atomic and molecular), outflowing or not from galaxies, and the impact of these winds on the efficiency of star formation, remain poorly constrained by observations. **JWST data will allow us to study at very high spatial resolution the energetics of the warm molecular gas through H₂ line spectral mapping.** In particular, one of the exciting possibilities is the study of the kinematics and physical state of the gas in the circum-nuclear disk and the torus, enabling us to see *whether molecular gas is entrained in the flow right from the very small scales, close to the supermassive black hole, or formed further out as a result of gas cooling.* JWST H₂ data will give us access to the gas dissipation rate and excitation, and thus will allow us to link the AGN activity and the turbulent dissipation.

Methodology: To advance our understanding of the regulation of the gas content in galaxies, both observational evidence of signatures of turbulence, as well as a physical model of gas cooling and energy dissipation are needed. In the following we detail the methodology planned to achieve the two main science objectives (observational and theoretical) of this PhD project.

1. Numerical modelling: The formation and excitation of molecular hydrogen in a turbulent multiphase medium will be modeled with 3D numerical simulations. The simulations will be configured to follow a large-scale shock propagating in a diffuse medium. The goal will be to analyze the fragmentation of the gas into small cold clouds and the formation, excitation, and survival of H₂, induced by such a shock. The simulations will be obtained using a recent development of the RAMSES code which include the chemistry and cooling of multiphase gas (Bellomi et al. 2020). New physical processes will be implemented into RAMSES to fully understand the link between large scale dissipation and phase transition. Depending on the interest of the student we will focus the project on the numerical development or the direct analysis of the H₂ spectral data (see below).

2. Observations: **The PhD student will contribute to the interpretation of datasets from JWST observations,** namely MIRI MRS & NIRSPEC IFU spectral-imaging of nearby galaxies with AGN and starburst-driven outflows. P. Guillard is co-PI of this program, whose sources are well-known for the extreme brightness of their H₂ lines (Ogle et al. 2010), which, with JWST, will be resolved spatially and spectrally. Building on our experience in interpreting Spitzer Telescope data, this is a unique opportunity to develop this expertise in the context of active galaxies and galaxy interactions. The student will lead the scientific exploitation of the H₂ spectral data, which will make it possible to trace the mass, kinematics and the excitation of the molecular gas in the outflows (Alvarez-Marquez et al. 2022).

Why is this PhD project relevant for the “Physique des Infinis” initiative? This thesis fits nicely within the scientific framework of the IPI, precisely because we propose to tackle the long-standing issue of the feedback loop regulating the gas content of galaxies, from an original observational and theoretical perspective. Indeed, the proposed PhD project connects the microphysics and chemistry at very small scales (turbulent dissipation at sub-parsec scales) to the study of the energetics of the large scale gas (kpc) reservoirs impacted by supermassive black holes in active galaxies.

Thesis supervision and collaborations: The PhD student will work with a team of astrophysicists from IAP and ENS, involved in several JWST proposals where H₂ will be observed in various astrophysical contexts and on a wide range of physical scales. The PhD candidate will benefit from this rich environment and will contribute to the team expertise. The project builds on our recognized expertise in modelling of the interplay between the dynamics, the physics and chemistry of interstellar matter, in particular H₂. The supervisors:

- **Pierre Guillard** ([ADS link](#)) studies the physics of galaxies (stars, gas, dust) and is a member of the JWST MIRI instrument Science and Test teams, P.I. of the commissioning activities related to the Point Spread Functions of the MIRI imager, and co-P.I. of a Guaranteed Time Observation project on nearby galaxies. He also has experience with photo-ionization models and shock models to explore the physics of cooling and to predict observables such as H₂ spectral lines. He has co-supervised 2 thesis (N. Cornuault, 2014-2017, 30%, and Suma Murthy 2018-2021, 50%) and 4 postdocs at 50%.

- **Benjamin Godard** ([ADS link](#)) is an expert of the numerical modeling of the coupling between interstellar chemistry and magnetohydrodynamics, radiative transfer, and the interpretation of spectroscopic molecular data. He is main developer of the publicly available **Paris-Durham shock code** (<https://ism.obspm.fr/shock.html>). He has supervised 1 thesis (E. Bellomi, 2017-2020) and co-supervised 3 postdocs at 80, 50, 20%.

Provisional calendar over the 3 years

Year 1: Bibliography, understanding of the subject - Getting familiar with the RAMSES code, setting up the simulation.

Year 2: Analysis of the simulated data - Interpretation of the JWST H₂ line data - start of writing of the first paper(s) and follow-up proposals.

Year 3: finishing up paper(s) - start of data analysis and interpretation of follow-up data if successful - thesis manuscript and completion.

PhD candidate profile: We seek a highly-motivated student with good programming skills (mostly python and Fortran) and interests in the physics of interstellar matter and numerical experiments

Short list of references:

Guillard, P., Boulanger, F., Pineau des Forêts, G., & Appleton, P. N. 2009, A&A, 502 — Ogle et al. 2010, ApJ, 724, 1193 — Álvarez-Márquez, J.; Labiano, A.; Guillard, P. A&A 2022, in press — Bellomi et al. 2020, A&A, 643A, 36B — Godard, B. et al. 2023 A&A, 669, 74 — Falle et al. 2020, MNRAS, 492, 448