Simulating interstellar icy grains in the laboratory

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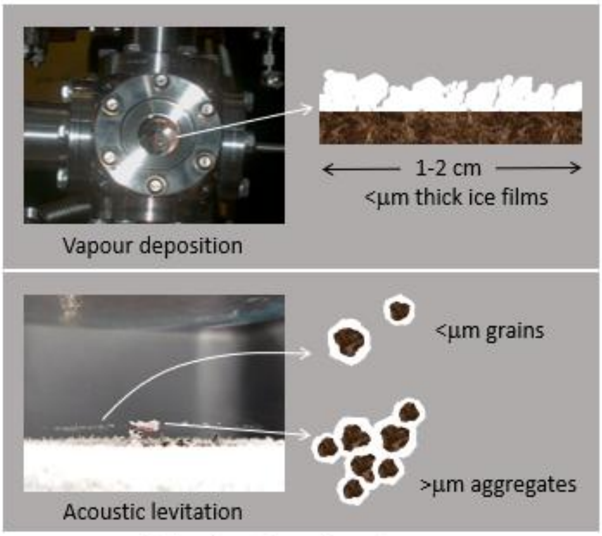
JWST NIRCam image of Rho Ophiuchi star forming region
(Credit: NASA, ESA, CSA, STScI, Kalus Pontoppidan)



Laboratory icy grain analogues

Project highlights:

- *Why this project matters:* This project tackles a central challenge in astrochemistry: understanding how molecular complexity emerges in star-forming regions and contributes to the chemical precursors of life. It directly supports the interpretation of James Webb Space Telescope (JWST) infrared ice spectra, bridging observational astronomy with laboratory molecular physics. By developing more representative interstellar ice analogues, the project fills a critical gap in current experimental data and modelling approaches.
- *What you'll achieve:* Develop realistic laboratory analogues of interstellar icy grain mantles and acquire high-resolution infrared and ultraviolet spectra to reveal how ice composition, morphology and scattering effects influence spectral features. These results will directly support the interpretation of JWST ice spectra and provide benchmark data for astrochemical models.
- *Training and development:* Gain hands-on experience with cryogenic systems, acoustic levitation, in situ spectroscopy and synchrotron beam time. Develop skills in experimental design, data analysis and collaborative research.
- *Collaborations and connections:* This cross-disciplinary project offers opportunities to engage with astronomers involved in JWST observations, molecular physicists, atmospheric physicists and beamline scientists, creating a direct link between laboratory experiments and space-based observations.

Project description:

Dense molecular clouds are the birthplaces of stars and planetary systems. Within these frigid (<10 K), dense regions, ice-coated dust grains act as microscopic laboratories, driving surface chemistry, facilitating gas-grain interactions, and ultimately becoming part of emerging planetary systems. These icy mantles, composed of simple molecular solids (H_2O, NH_3, CH_4, CO_2, CO and CH_3OH), undergo thermal and non-thermal processing (via photons, ions and electrons) during cloud collapse and protoplanetary disc formation, leading to the formation of complex organic molecules, enriching the protostellar environments[1]. Understanding this chemical evolution is key to tracing the origins of molecular complexity – and, ultimately, life.

Recent high-resolution infrared absorption spectra from the James Webb Space Telescope (JWST) are revealing exciting new details about ices in dense molecular clouds[2]. However, interpreting these observations requires laboratory spectra measured under controlled conditions that accurately simulate interstellar environments. Astrochemical models rely heavily on empirical input from laboratory studies, yet current datasets are limited. Most laboratory spectra are measured through ice films grown on flat cm-sized substrates – unrepresentative of microscopic 3D 'fluffy' interstellar ice grains. Scattering effects, which distort interstellar molecular ice band profiles are strongly influenced by grain size and aggregation[3]. These scattering-induced distortions, clearly observed in astronomical spectra, have not yet been reproduced or characterised in the laboratory.

Project description:
This project will investigate the physical and chemical properties of interstellar ice analogues across macroscopic and microscopic scales using two complementary approaches:

(a) *Vapour deposited films:* Using *in situ* infrared spectroscopy (Molecular Astrophysics Lab, OU) and vacuum ultraviolet spectroscopy (ASTRID2 synchrotron facility, University of Aarhus, Denmark), this part of the project will probe the vibrational and electronic states of pristine and processed molecular ice films under simulated interstellar conditions, characterising compositional and morphological effects[4].

(b) *Acoustically levitated aerosols:* Icy particles will be suspended in an ultrasonic acoustic field[5] and spectroscopically analysed to explore how particle size, aggregation and processing affect spectral profiles. Comparing these spectra with those from thin films will help disentangle compositional and morphological effects from optical scattering (Mie and Rayleigh).

The combined IR and VUV study will produce benchmark spectra for interpreting JWST observations and refining astrochemical models

We seek a motivated candidate with interests in molecular physics, physical chemistry or astrochemistry, and a willingness to develop a range of laboratory skills. The successful candidate will work in a supportive laboratory research environment within the School of Physical Sciences, contribute to beam time proposals and participate in experimental campaigns at international facilities. The project offers collaboration with astronomers (with access to JWST ice data), theoretical and experimental physicists and chemists, planetary scientists, and aerosol physicists, fostering interdisciplinary knowledge exchange across astrochemistry, atmospheric science, and molecular physics.

References:

1. Chen, Y. *et al.* JOYS+: The link between the ice and gas of complex organic molecules-Comparing JWST and ALMA data of two low-mass protostars. Astronomy & Astrophysics, 690, p.A205 (2024).
2. McClure, M.K. *et al.* An Ice Age JWST inventory of dense molecular cloud ices. Nature astronomy, 7(4), pp.431-443 (2023).
3. Dartois, E. *et al.* Spectroscopic sizing of interstellar icy grains with JWST. Nature astronomy, 8(3), pp.359-367 (2024).
4. James, R.L. *et al*. Systematic investigation of CO_2: NH_3 ice mixtures using mid-IR and VUV spectroscopy–part 2: electron irradiation and thermal processing. RSC advances, 11(52), pp.33055-33069 (2021).

5. Mason, N.J. *et al.* The spectroscopy and chemical dynamics of microparticles explored using an ultrasonic trap. Faraday discussions, 137, pp.367-376 (2008).

Qualifications required: BSc 2:1 or a MSc in a relevant discipline. Ideally a student with a 4-year integrated Masters level qualification in Physics, Astronomy or Chemistry.