Investigating Interstellar Ice Analogues with LISA and FELIX

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Free Electron Lasers for Infrared eXperiments

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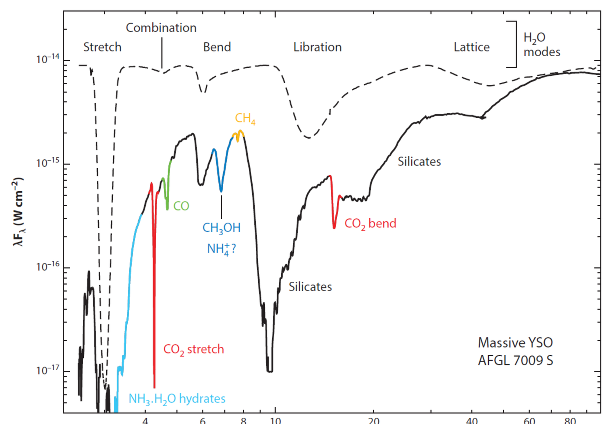
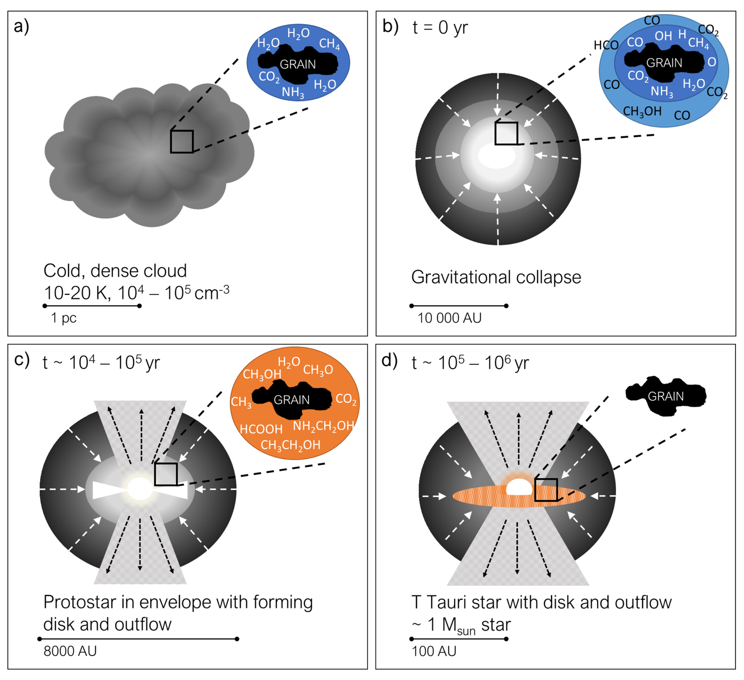
Exploring interstellar ices

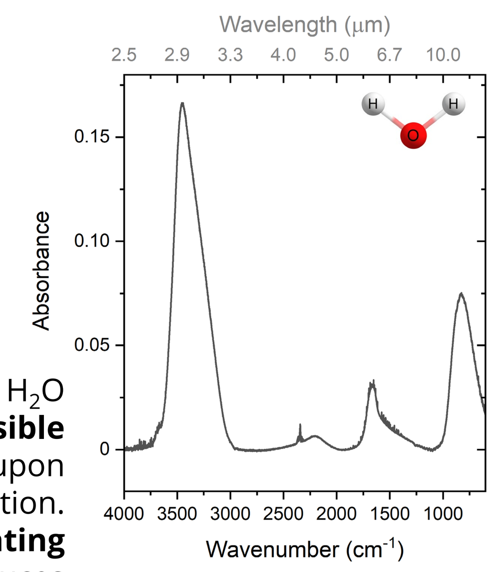
Interstellar ices are postulated to play an important role in **interstellar chemistry**, such as the formation of the most abundant molecule H_2 [1]. Only 6 molecular species have so far been detected in the solid state - **H_2O, CO, CO_2, CH_3OH, NH_3 and CH_4** [2]. However, it is suggested that there are many more species present in these icy mantles, such as complex organic molecules (COMs) and prebiotic species. The recent launch of the **James Webb Space Telescope (JWST)** targets the detection and further exploration of these species and will inspire **a new "ice age"** in astrochemical research.





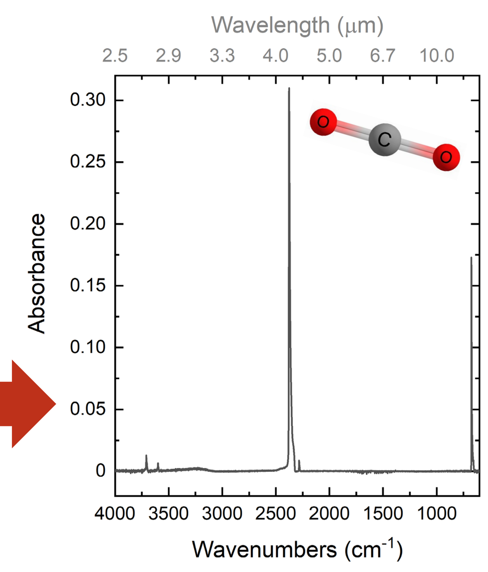
The **Laboratory Ice Surface Astrophysics (LISA)** chamber at the **free electron laser (FEL) facility FELIX** has been designed to study the effect of the **release of vibrational energy** in the **bonding network of ices** of interstellar relevance [3,4]. By employing the wide tunability and high intensity of the FELs at FELIX, ices grown in the ultra-high vacuum chamber of LISA are selectively **irradiated on- and off-resonance** in the **mid-infrared (MIR) range** at temperatures below **20 K**. Infrared radiation is **ubiquitous in space**, but the release of vibrational energy in the ice layers can also result from **exothermic chemical reactions** in these layers. Then, understanding how this kind of energy can be taken up and dissipated in structure of an interstellar ice is key in **investigating grain-surface reactions**. We aim to study all 6 molecular species, as well as mixed and layered ices, such as the **CO_2:H_2O mixtures** shown here.

Systematic survey of mixed H_2O:CO_2 ices



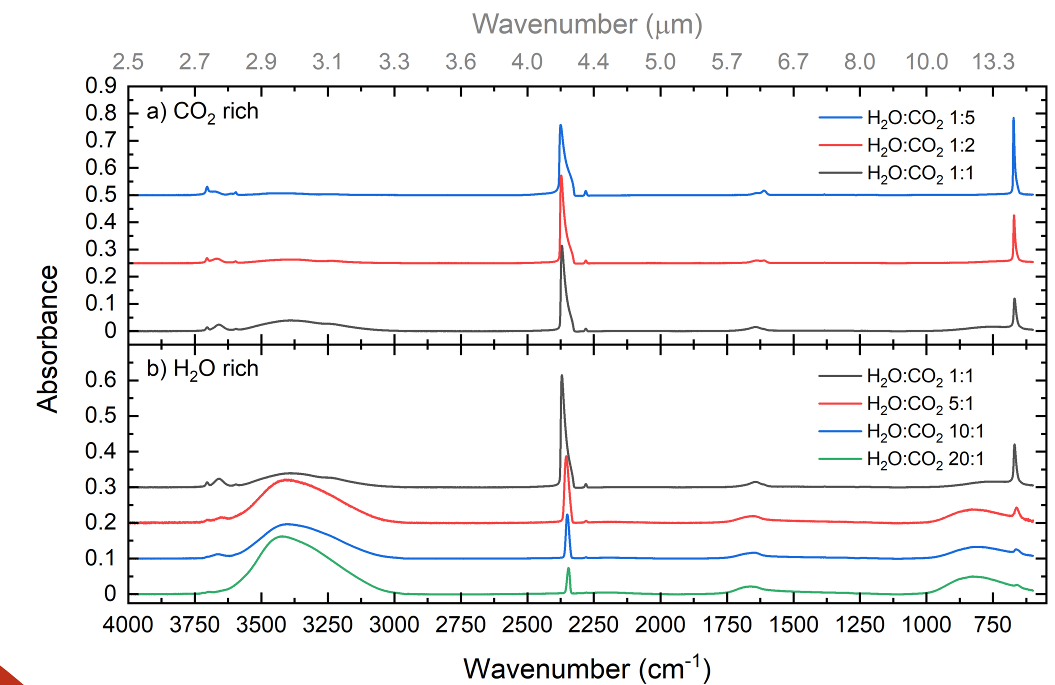
Pure amorphous H_2O shows **irreversible restructuring** upon resonant irradiation. **Local heating** induces crystallization

[4] Noble *et al.*, *J. Phys. Chem. C* 2020. **124** (38) 20864–20873



Pure amorphous CO_2 shows **irreversible restructuring** upon resonant irradiation

[3] Ioppolo, S. et al., *J. Mol. Spectrosc.* 2022. **385**, 111601-1 -111601-8.

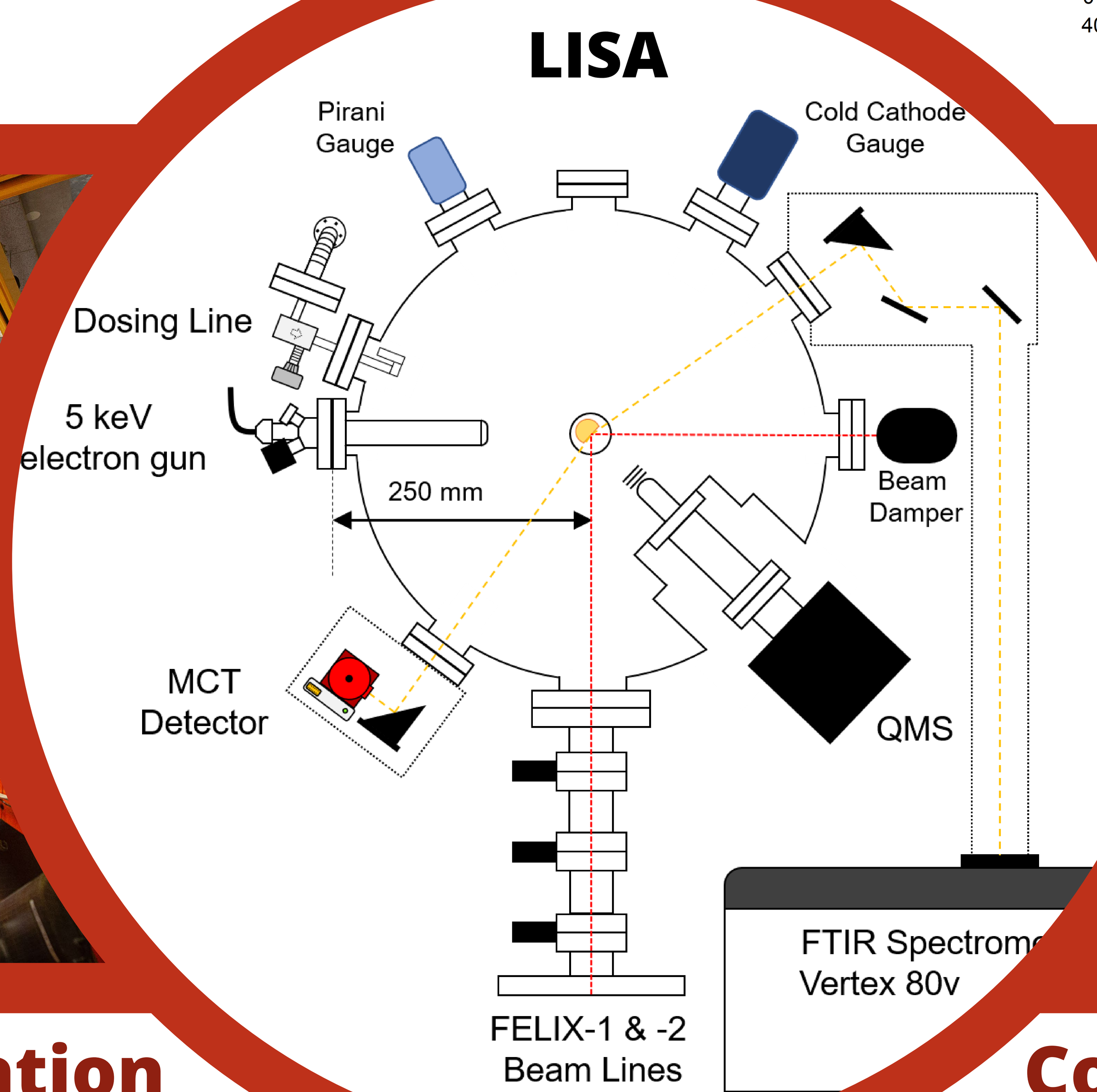


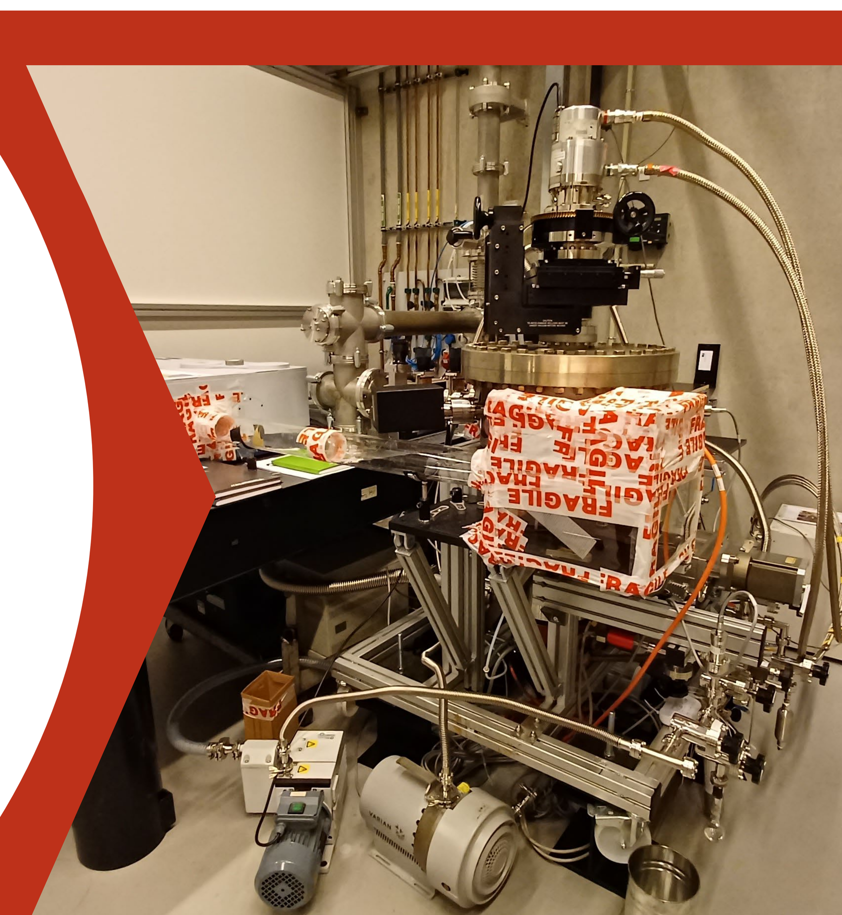
Reflection absorption infrared (**RAIRS**) spectra of a systematic selection of **H_2O:CO_2** mixing **ratios**

FELIX FEL-2

Spectral range	2.7 – 45 μm 3600 – 200 cm^{-1}
Micropulse rep. rate	25, 50 or **1000 MHz**
Macropulse rep. rate	**5** or 10 Hz
Macropulse energy at 1 GHz	< 200 mJ
Bandwidth	0.4 -5 %

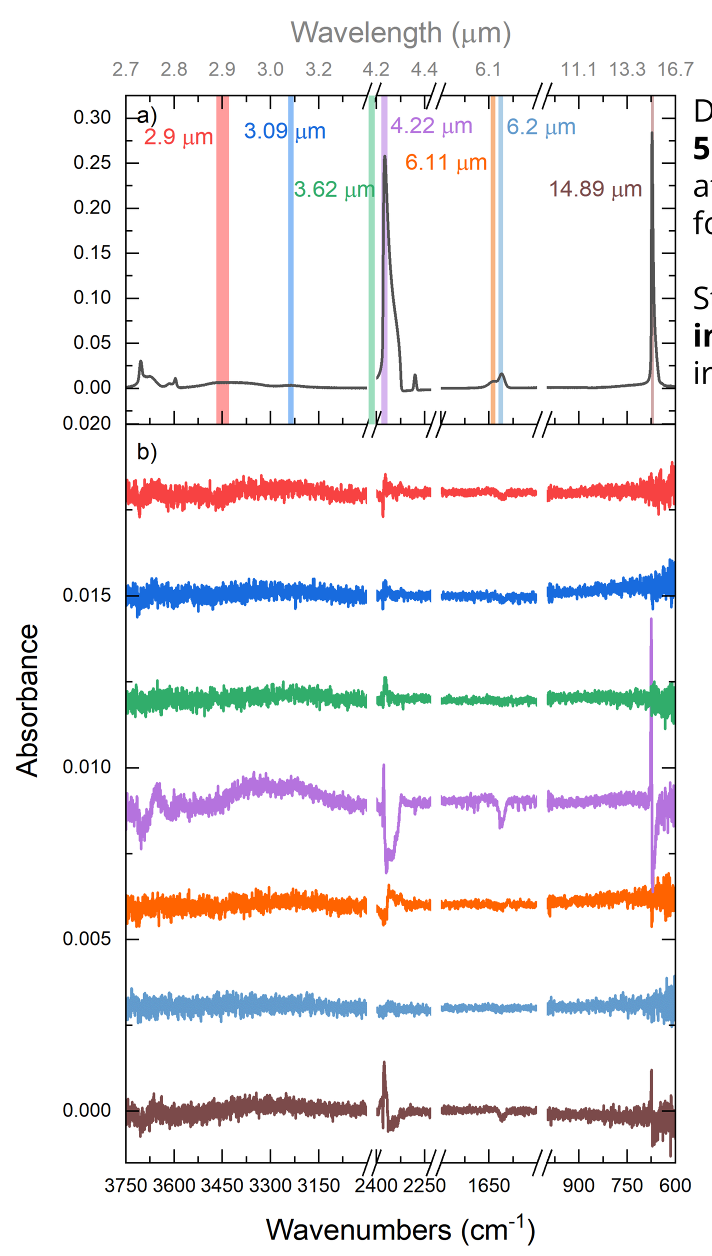
HFML-FELIX laboratory
Nijmegen, The Netherlands





Base pressure	1·10^{-9} mbar
Temp. range	18 – 300 K
Substrate	Gold coated; optically flat
RAIRS angle	13°

Selective infrared FEL irradiation



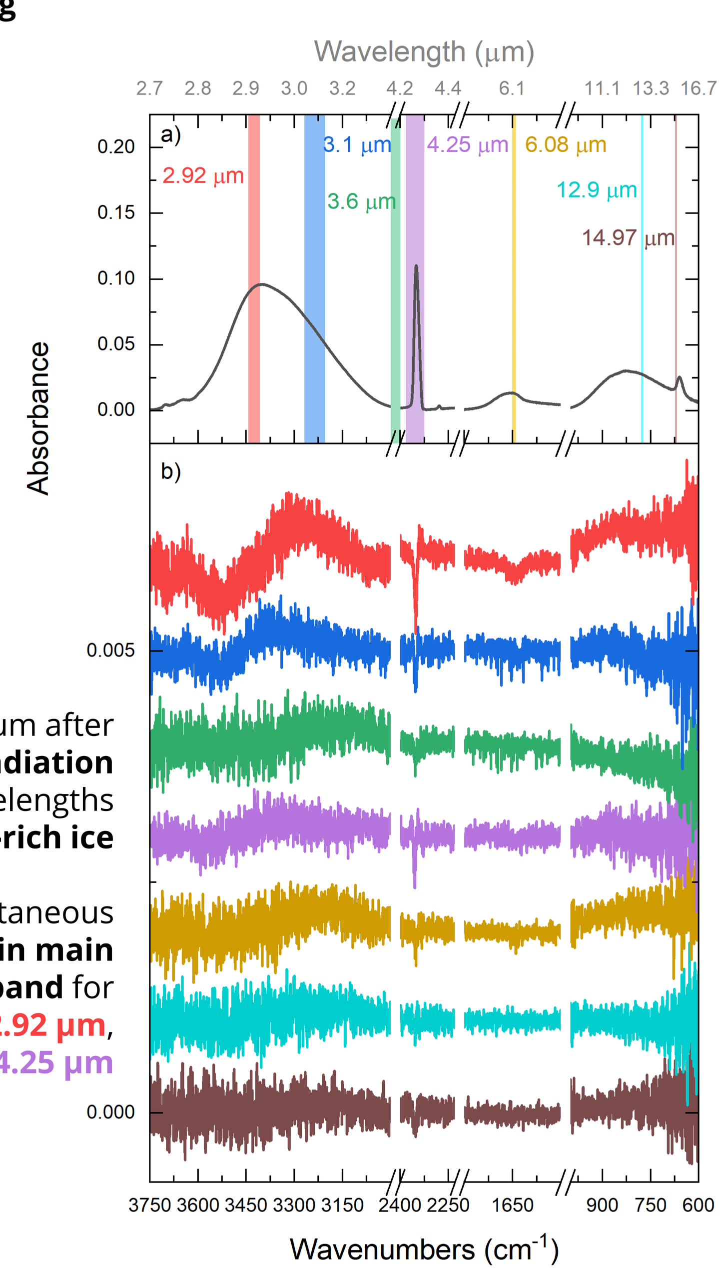
Difference spectrum after **5 minutes of irradiation** at resonant wavelengths for a **CO_2-rich ice**

Strongest restructuring in main CO_2 band for irradiation at **4.21 μm**

Irradiation at **3.6 μm** is **off-resonance**

H_2O:CO_2 1:5

H_2O:CO_2 10:1



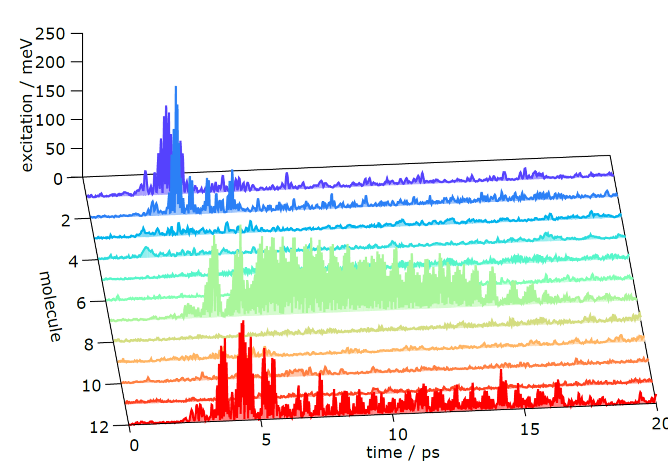
Difference spectrum after **5 minutes of irradiation** at resonant wavelengths for a **H_2O-rich ice**

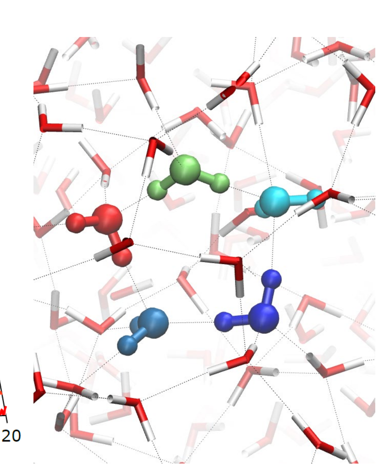
Simultaneous **restructuring in main H_2O AND CO_2 band** for irradiation at **2.92 μm**, **3.1 μm** and **4.25 μm**

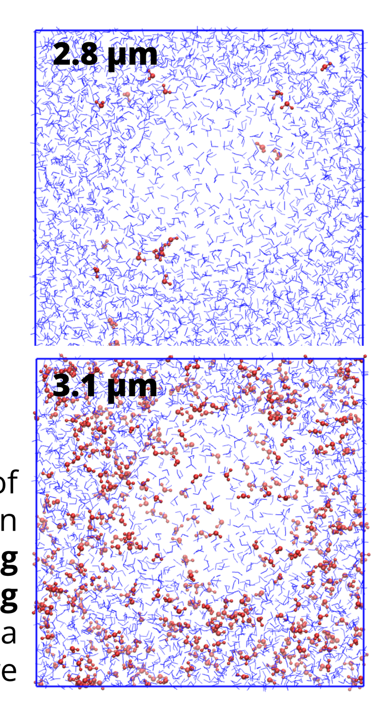
Conclusions and Outlook

- Clear indications of **irreversible structural changes** in H_2O:CO_2 ices **due to FEL irradiation** as opposed to thermal effects
- Restructuring **wavelength dependent**, i.e. more H_2O, more effect with 2.9 μm
- Need **theory** to link the macroscopic effects to microscopic processes
- Push experiments to **time-dependent studies** of the structural changes

Classical **simulations of energy dissipation** in porous amorphous solid water.







Effect of irradiation on **H-bonding surrounding** around a pore

References

[1] Hollenbach, D. and E.E. Salpeter, *Astrophys. J.* 1971. **163**, 155.
[2] Boogert, A.C.A. et al., *Annu Rev Astron Astr*, 2015. **53**(1), 541-581.
[3] Ioppolo, S. et al., *J. Mol. Spectrosc.* 2022. **385**, 111601-1 -111601-8.
[4] Noble, J.A. et al., *J Phys Chem C*, 2020. **124**(38), 20864-20873.

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