

# HighNESS General Meeting

Work Package 2 - Software Development

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# HighNess

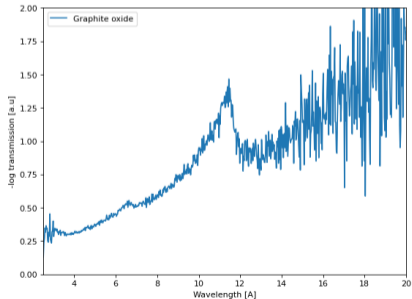
## Current status

- D2.1 (nanodiamonds) and D2.2 (magnesium hydride) deliverables finished.
- Finalizing work on the nano-diamonds particles: molecular modelling. Manuscript in preparation.
- Focus on intercalated graphites (D2.3) and the clathrate hydrates (D2.4).
- All this work is supported by NCrystal developments.



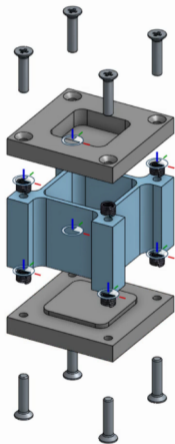
## Deliverable D2.3 (Intercalated graphite)

- Work has primarily focused on measurements at PSI. Two experiments carried out, third to follow in July.
- Second experiment improved drastically the background making it possible to resolve the Bragg edge in graphite oxide around 12 angstroms.



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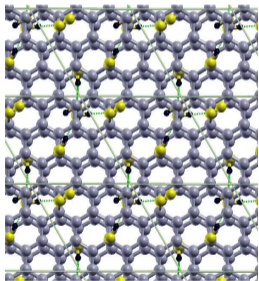
PSI experiment



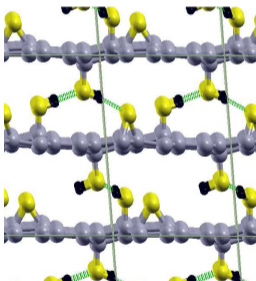
- Sample appears highly textured, we have designed a new sample holder for the follow-up measurement
- Manufacturing in progress.
- Aim to measure the samples across the three different orientations.



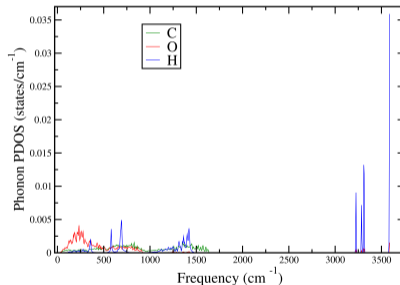
- Modelling in progress, with DFT simulations from UNIMIB



Top view

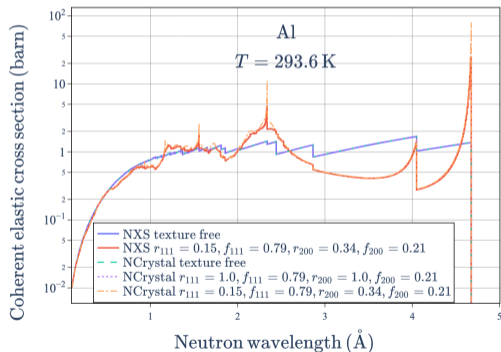


Side view



PDOS

- Implemented March-Dollase texture model as NCrystal plugin:

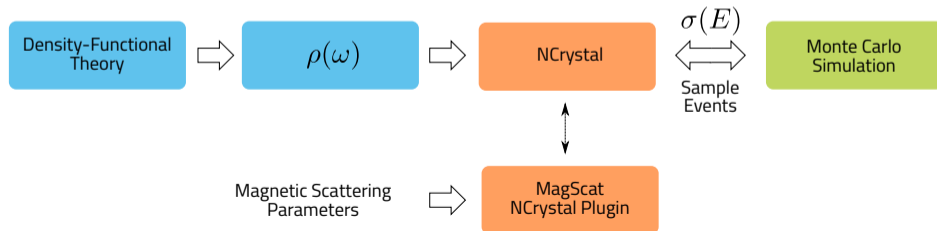


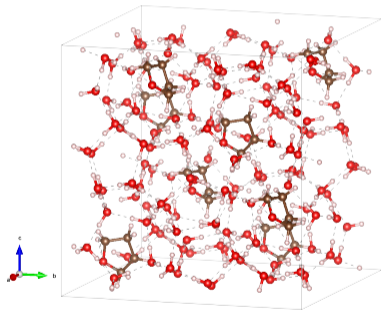
- Good agreement obtained between the developed plugin and the NXS code [1].

## Deliverable D2.4 (Clathrate Hydrates)

Clathrate hydrates are ice-like compounds having a cage structure. Small molecules such as methane can be enclathrated in the cage, stabilising the structure.

- Tetrahydrofuran (THF/TDF)-containing clathrate hydrates: low energy modes
- Oxygen-containing clathrate hydrates: neutron inelastic magnetic scattering

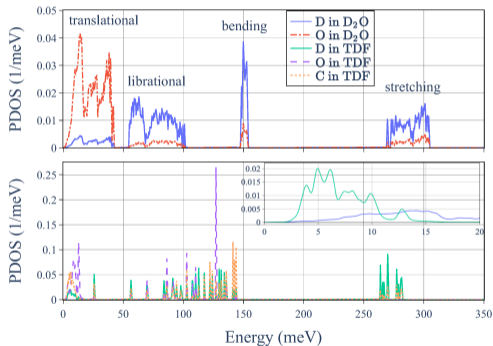
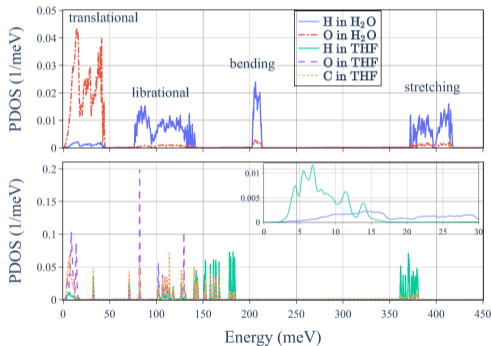




- Crystalline structure of THF-containing clathrate hydrate (structure II) optimised with DFT calculations
- Unit cell having 136 water molecules and 8 THF molecules inserted in large cages
- Phonon DOS computed using CP2K and phonopy

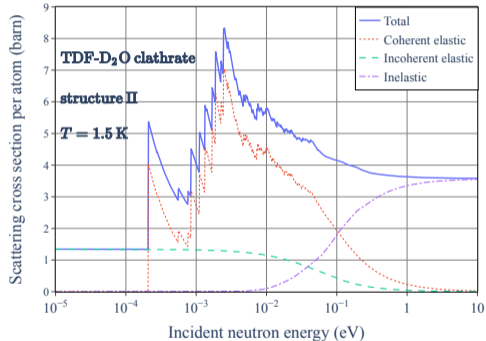
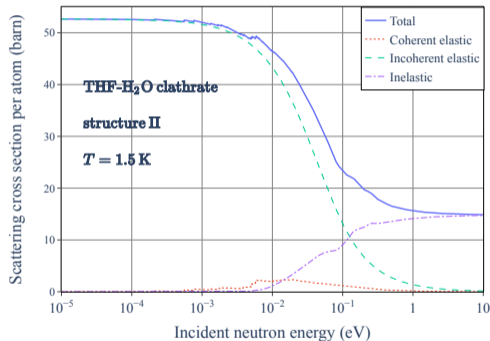


## DFT Simulations - phonon density of states

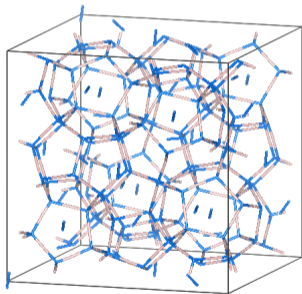


Low energy modes of the guest molecules make the TDF-clathrates a promising cold moderator candidates.

## NCrystal Calculations - neutron scattering cross sections



The theoretical neutron scattering cross sections serve to compare against existing or future experimental data.



- Crystalline structure obtained from DFT calculations
- Unit cell composed of 136  $D_2O$  and 24  $O_2$  enclathrated in both large and small cages

## Neutron slowdown by paramagnetic oxygen

Based on Zimmer's paper [2], the neutron magnetic scattering kernels or dynamic structure factors  $S_{\text{mag}}(Q, \omega)$  are derived:

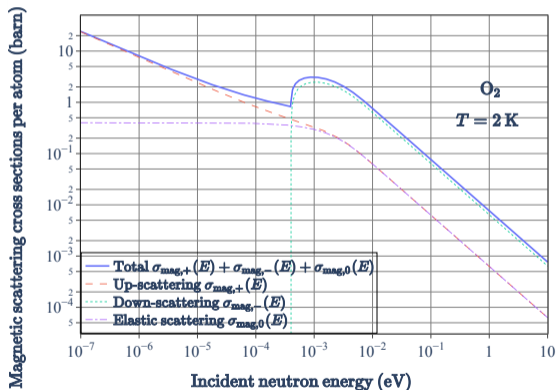
$$\frac{d^2\sigma_{\text{mag}}}{d\Omega dE'} = b_m^2 \left( \sqrt{\frac{E'}{E}} S_{\text{mag},\pm}(Q, \omega) + S_{\text{mag},0}(Q, \omega) \right), \quad (1)$$

where

$$S_{\text{mag},\pm}(Q, \omega) = \exp \left( -(\langle u^2 \rangle + \frac{\ln(2)}{\Gamma_{\text{mag}}^2}) Q_{\pm}^2 \right) g_{\pm}(T) \delta(\hbar\omega \pm D), \quad (2)$$

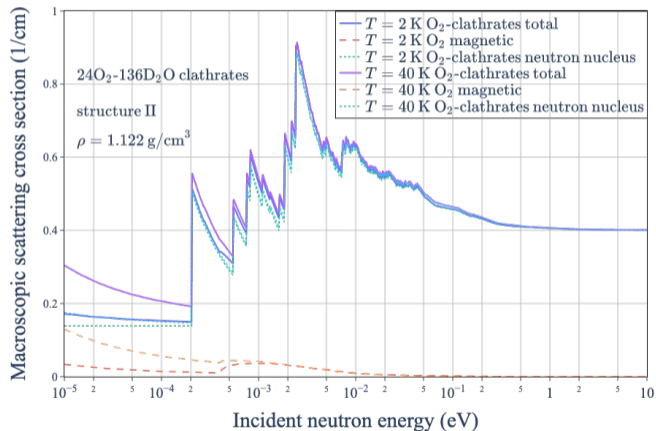
and

$$S_{\text{mag},0}(Q, \omega) = \exp \left( -(\langle u^2 \rangle + \frac{\ln(2)}{\Gamma_{\text{mag}}^2}) Q_0^2 \right) g_0(T) \delta(\hbar\omega). \quad (3)$$



- Magnetic cross sections generated by the developed plugin `ncplugin-MagScat`

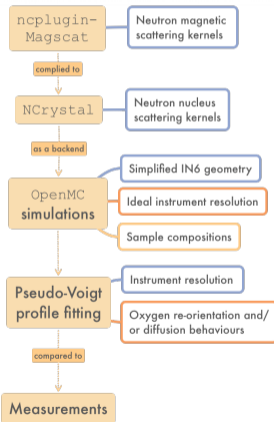
## NCrystal Calculations - Neutron scattering cross sections



- Cross sections calculated for 136 D<sub>2</sub>O + 24 O<sub>2</sub>
- Mean free path near to 25 cm for magnetic down-scattering at 2 K

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## Monte-Carlo simulations of measurements

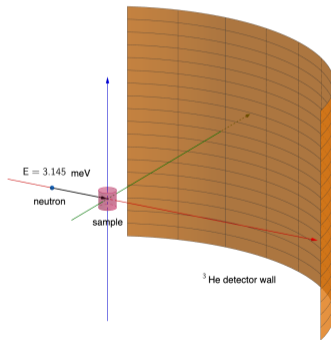


OpenMC [3] Monte-Carlo simulations on experiments performed by Chazallon et al. [4] on O<sub>2</sub>-clathrates and Renker et al. [5] on O<sub>2</sub>-C<sub>60</sub>.



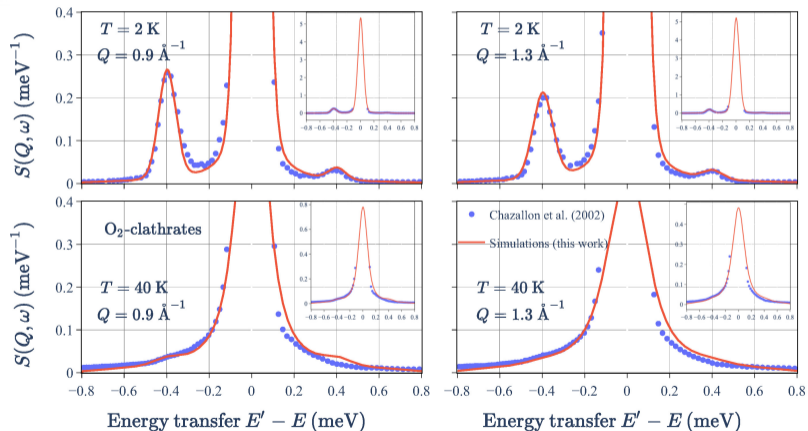
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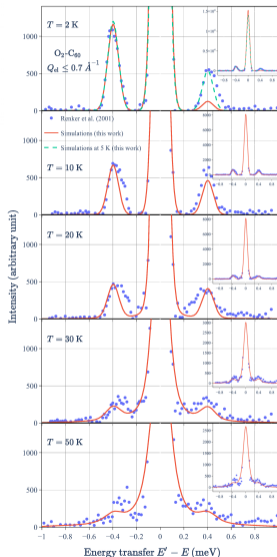
Inelastic neutron scattering measurements on time-of-flight spectrometer IN6 at ILL



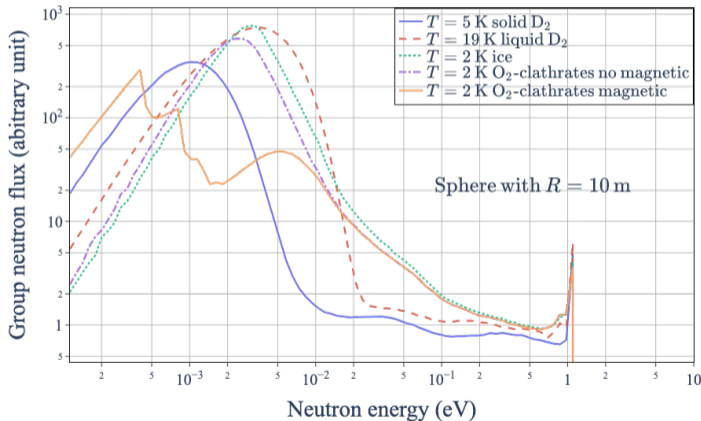


## Monte-Carlo simulations on O<sub>2</sub>-clathrates





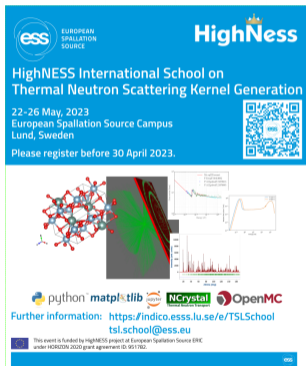
## Comparisons of neutron spectra



- Preliminary results
- Further optimisation of configuration by Blahoslav Rataj from WP4 on going

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## Thermal Scattering School



The poster features a blue header with the ESS logo and the HighNESS logo. Below the header, the title and dates are listed. A QR code is positioned on the right side of the header. The main content area contains a molecular structure visualization, a 3D plot, and several line graphs. At the bottom, logos for Python, matplotlib, NumPy, NCrystal, and OpenMC are displayed, along with contact information and funding details.

ess EUROPEAN SPALLATION SOURCE HighNESS

HighNESS International School on  
Thermal Neutron Scattering Kernel Generation

22-26 May, 2023  
European Spallation Source Campus  
Lund, Sweden

Please register before 30 April 2023.

python matplotlib NumPy NCrystal OpenMC

Further information: <https://indico.ess.lu.se/e/TSLSchool>  
[tsl.school@ess.eu](mailto:tsl.school@ess.eu)

This event is funded by HighNESS project of European Spallation Source ERIC  
under HORIZON 2020 grant agreement ID: 951782.

- First school of its kind.
- Over 30 participants registered from around the world.
- It will cover theory of neutron scattering, and implementations using open source tools.



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## Summary

- Deliverables D2.1 and D2.2 have been finalized.
- Implementation of magnetic scattering model in addition to molecular modeling simulations of clathrates with DFT. Manuscript under preparation.
- Work on graphite compounds is underway. Two experiments carried out, with a followup in July. Texture model implemented and DFT simulations in progress.



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## References



Mirko Boin.

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