HighNess

HighNESS General Meeting

Work Package 2 - Software Development

D. Di Julio, J.I.Marquez Damian, Marco Bernasconi, Davide Campi, Giuseppe Gorini, Thomas Kittelmann, Sara Laporte, and Shuqi Xu

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Main Aims of Work Package

Development of software to describe low-energy neutron transport in reflectors and moderator materials.

Tasks:

2.1. Develop models for magnesium hydride, nanodiamonds, intercalated graphite, and clathrate hydrates. Models will be implemented in NCrystal to be used in Geant4, MCNP, PHITS, or OpenMC.

2.2. Develop molecular modelling techniques, such as molecular dynamics and density functional theory, in order to provide input to the models in task 2.1.

Deliverables:

D2.1. Report and simulation software for nano-diamonds (M12)

D2.2. Report and simulation software for MgH_2 (M12)

D2.3. Report and simulation software for intercalated graphite (M34)

D2.4. Report and simulation software for clathrate hydrates (M34)

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Current status

- D2.1 (nanodiamonds) and D2.2 (magnesium hydride) deliverables finished.
- Work published in NIM A (NJOY+NCrystal paper) and presented at AccApp 2021 and Nuclear Data 2022.
- Finalizing work on the nano-diamonds particles: molecular modelling.
- Work has started on the clathrate-hydrates: Molecular modelling and implementation of magnetic scattering.
- Experiment at PSI on intercalated graphites, followup proposal submitted.
- All this work is supported by NCrystal developments.

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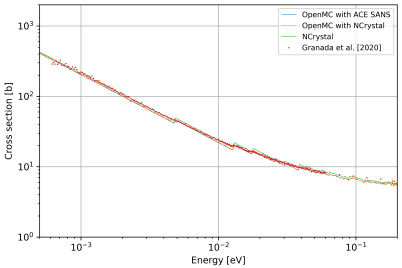
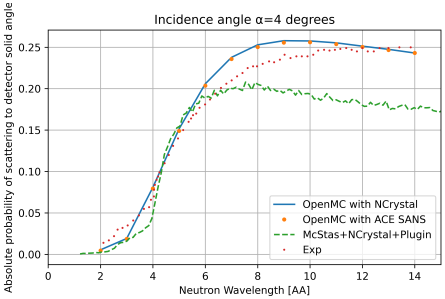
Results D2.1 (Nanodiamonds)

- Implemented as an ACE library + SANS subroutine and by direct call of NCrystal with the nanodiamond plugin.
- Based on molecular modelling including the finite-size effects of the nano-diamonds





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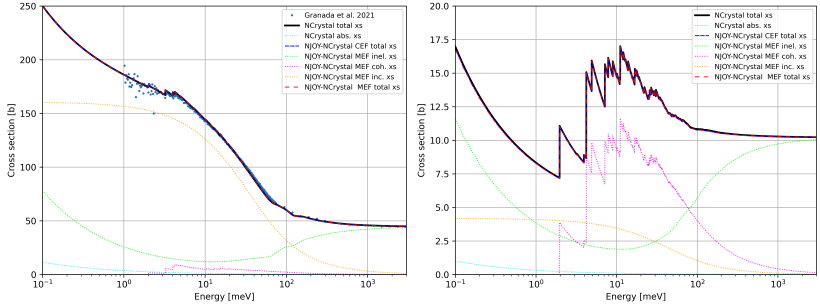
Results D2.2 (Magnesium Hydride)

- NJOY+NCrystal mixed elastic (MEF) and current ENDF (CEF) formats.
- Phonon spectrum computed from DFT simulations by U. Milano-Bicocca.



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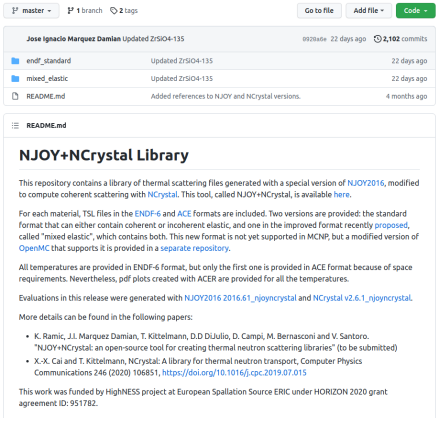
NJOY+NCrystal Library

- New developments led to creation of the largest TSL library to date. A total of 213 new evaluations.
- Provides extensive benchmarking for the methods developed in WP2.



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All developments are freely available online

They are hosted on Github, following the Data Management Plan:

- OpenMC+Ncrystal:
  `https://github.com/highness-eu/openmc/tree/mixed_ncrystal`
- NCrystal nanodiamonds plugin:
  `https://github.com/highness-eu/ncplugin-SANSND`
- NJOY+Ncrystal:
  `https://github.com/highness-eu/NJOY2016/tree/njoy_ncrystal`,
  `https://github.com/highness-eu/ncrystal/tree/njoy_ncrystal`
- NJOY+Ncrystal Library:
  `https://github.com/highness-eu/NJOY-NCrystal-Library`

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Deliverable D2.3 (Intercalated graphite)

- Creating scattering models and testing: Using NJOY+NCrystal.
- Measurements at PSI and follow-up proposal submitted with WP3.
- Survey of possible materials. Carbon / fluorine / oxygen intercalated compounds; C_{60}; Other compounds.
- Microscopic modelling by UNIMIB.

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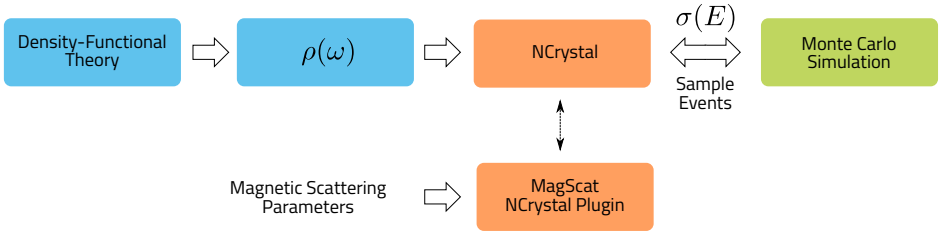
Deliverable D2.4 (Clathrate Hydrates)



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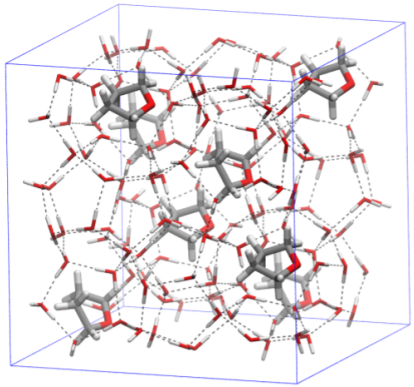
DFT Simulations



- Tetrahydrofuran (THF) SII hydrate model optimised with DFT
- THF occupies the large cages, unit cell has 136 water molecules and 8 THF molecules
- Phonon DOS computed using CP2K and phonopy

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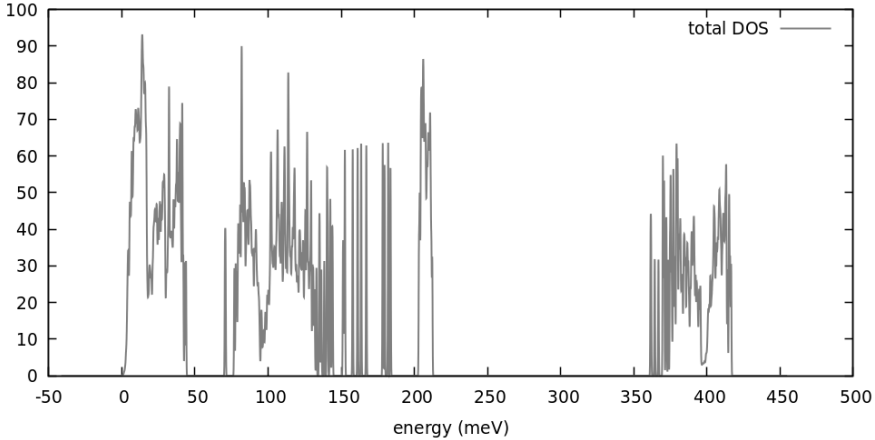
DFT Simulations - phonon density of states



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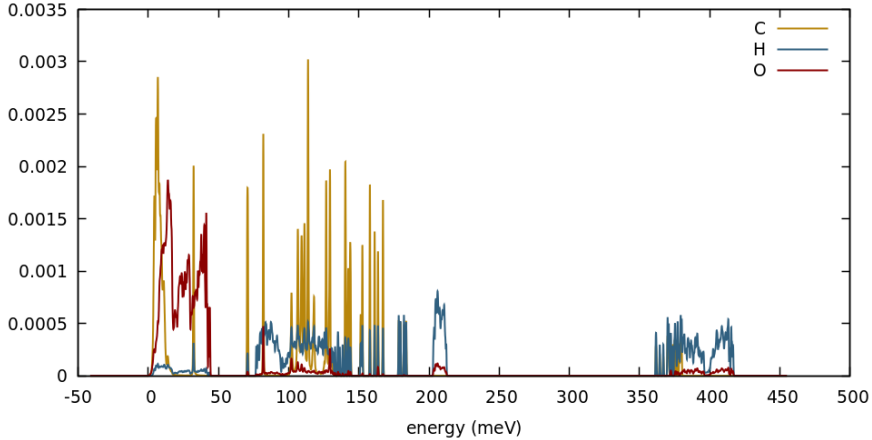
DFT Simulations - projected density of states



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Neutron slowdown by paramagnetic materials

It is theoretically verified the production of VCN by paramagnetic materials encaged in clathrate hydrates, and deuterated O2-clathrate hydrates appear particularly promising (Zimmer 2016). The double differential magnetic scattering cross section for unpolarized neutrons is given by:

Magnetic form factor

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega \mathrm{d}E'} = b_{\mathrm{m}}^2 \frac{k'}{k} \exp(-2W)|F(\kappa)|^2 \times \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \left(\frac{1}{3}\langle S^+S^-(t) + S^-S^+(t)\rangle + \frac{2}{3}\langle S_z^2\rangle \right) \exp(-i(E-E')t/\hbar)\mathrm{d}t.$$

Inelastic (down & up-scattering)

Elastic

Oliver Zimmer. Phys. Rev. C, 93:035503, Mar 2016.

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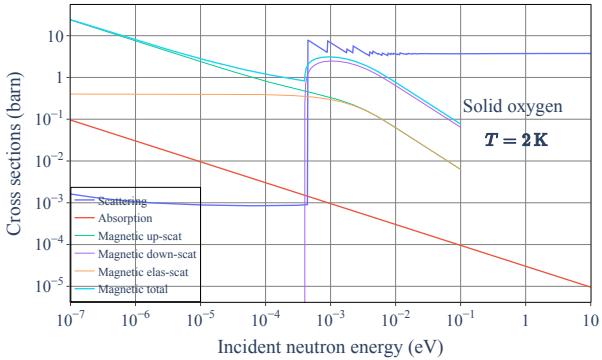
Magnetic cross sections of solid oxygen

Solid oxygen ($Pm\bar{3}n$) is investigated. The cross sections are calculated by using NCrystal-3.0.0+MagScat plugin.



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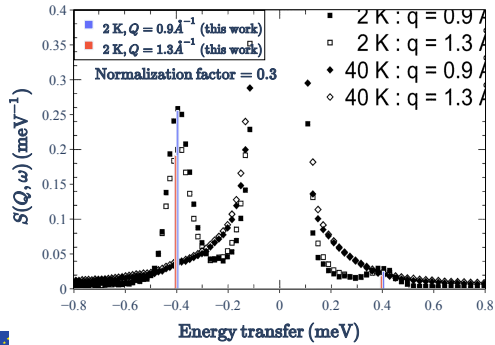
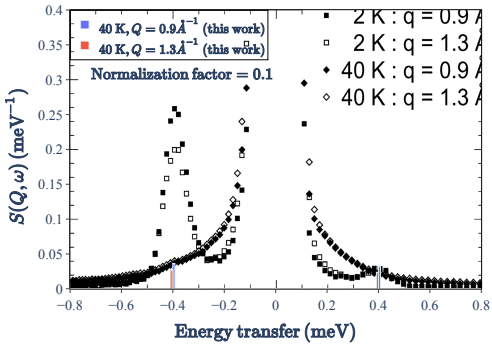
Investigation of Chazallon's experiments

Though the peaks at around 0.4 meV are tentatively attributed to crystal field effects by the authors, we reproduce correctly with the magnetic formulae derived by Zimmer. Monte-Carlo simulations by using OpenMC+NCrystal are ongoing.





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Chazallon et al. Phys. Chem. Chem. Phys., 4:4809–4816, 2002.

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NCrystal 3.0

- Improved data library: 131 materials
- Framework support for multiphase materials.
- Framework for SANS physics, including utilities for easier handling of SANS plugins.
- Improved integration with McStas, supporting McStas 2.x and 3.x and supporting NCrystal materials in McStas Union. Thanks to collaboration with Mads Bertelsen.
- Going forward: improving sampling and biasing for UCN and VCN production.

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Summary

- Deliverables D2.1 ad D2.2 have been finalized.
- Software and data were released according to the data management plan and results were presented in a NIM A paper and the AccApp conference.
- Implementation of magnetic scattering model is ongoing in parallel to the molecular modelling simulations of clathrates with DFT
- Work on graphitic compounds has started. First experiment carried out with a followup proposal submitted for later this year.

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