EUROPEAN
SPALLATION
SOURCE

HighNESS - Work Package 2

Software Development

PRESENTED BY D. DI JULIO, J.I. MÁRQUEZ DAMIÁN

KICKOFF MEETING, 26-10-2020

HighNESS is funded by the European Union Framework Program for Research and Innovation Horizon 2020, under grant agreement 951782

Objectives:

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 hydrites. 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.

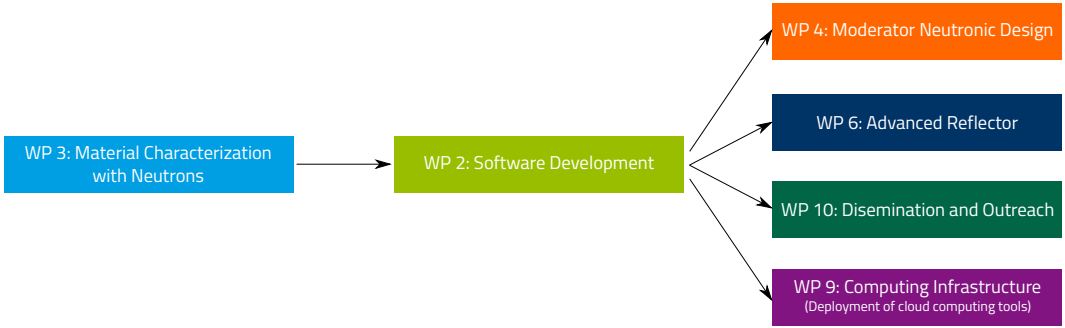
Deliverables:

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)


WP 3: Material Characterization with Neutrons
WP 2: Software Development
WP 4: Moderator Neutronic Design
WP 6: Advanced Reflector
WP 10: Disemination and Outreach
WP 9: Computing Infrastructure
(Deployment of cloud computing tools)

Human Resources

- Giuseppe Gorini
- Marco Bernasconi
- Davide Campi
- + postdoc to be hired by UNIMIB.

UNIVERSITÀ DEGLI STUDI DI MILANO BICOCCA

Spagnolatti, I., Mussi, A., Bernasconi, M. et al. Vibrational properties of C20-based solids. Eur. Phys. J. B 37, 143–148 (2004).

A. Ruckhofer, D. Campi, M. Bremholm, P. Hofmann, G. Benedek, M. Bernasconi, W. E. Ernst and A. Tamtögl, Terahertz Surface Modes and Electron-Phonon Coupling on Bi2Se3(111), Physical Review Research 2, 023186 (2020).

Mostafa Jamalipour, Zanini, L. and Gorini, G. Implementation of Neutron Reflection with Nano-Dispersed Media in Geant4. J. Synch. Investig. 14, S75–S78 (2020).

Campi, D., Bernasconi M., Benedek G. Phonons and electron-phonon interaction at the Sb(111) surface. Phys. Rev. B 86, 075446 (2012)

Human Resources

- Douglas Di Julio
- Thomas Kittelmann
- Jose Ignacio Marquez Damian
- Kemal Ramic

DiJulio, D.D., Lee, Y. J., Muhrer, G. Impact of crystallite size on the performance of a beryllium reflector. Journal of Neutron Research, vol. 22, no. 2-3, pp. 275-279, 2020

Cai, X.-X. and Kittelmann, T.NCrystal: A library for thermal neutron transport, Computer Physics Communications 246 (2020) 106851.

Granada, J. R, Márquez Damián, J.I, and Helman, C. Studies on reflector materials for cold neutrons.EPJ Web of Conferences, vol. 231, p. 04002. EDP Sciences, 2020.

Ramić, K. From Experiments to DFT Simulations: Comprehensive Overview of Thermal Scattering For Neutron Moderator Materials. PhD Thesis. Rensselaer Polytechnic Institute (2018).

Workflow

Task 2.2

Task 2.1

NCrystal

Molecular Dynamics (liquids)

DFT (solids)

Atomic Structure

Frequency Spectra

Magnetic Scattering

Incoherent Scattering

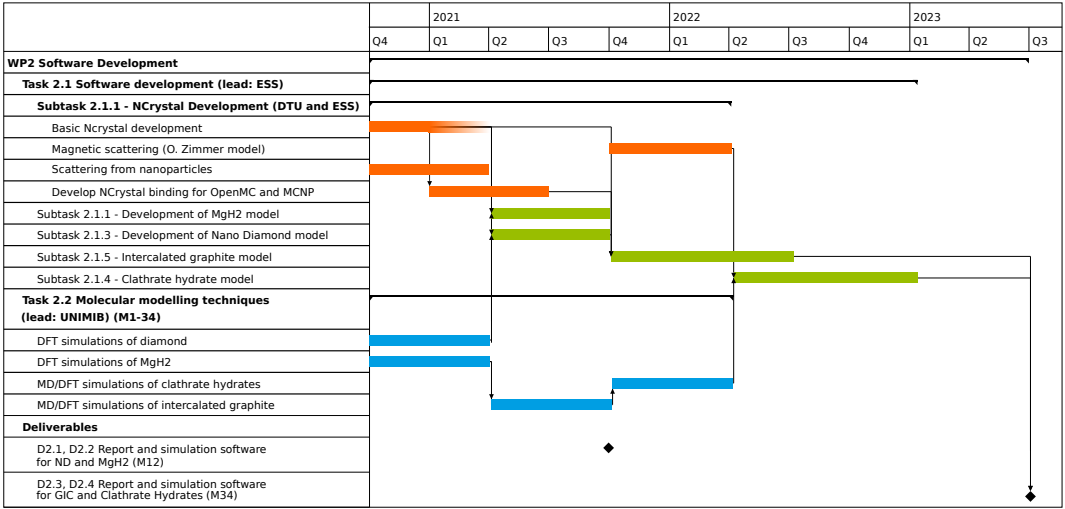
Bragg Scattering

Small Angle Neutron Scattering

Dynamic Structure Factor

Neutronic Monte Carlo Simulation (OpenMC, MCNP, PHITS, Geant4, McStas)

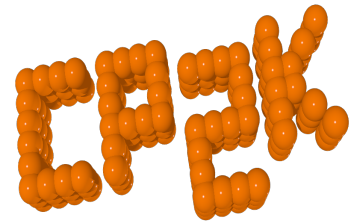
Preliminary Planning



Groundwork I

Simulation methods and codes at UNIMIB:

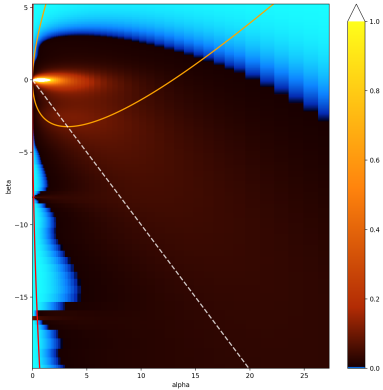
- Density Functional Perturbation Theory. Code: Quantum-Espresso
- Finite difference calculations of the dynamical matrix from supercell. Code: CP2k
- Vibrational density of states from velocity-velocity autocorrelation function within DFT molecular dynamics for strongly anharmonic systems. Code: CP2k
- Classical interatomic potentials (e.g. Tersoff-like) to compute phonon density of states for very large systems.Codes: LAMMPS, DL_poly.



Groundwork II

Status of NCrystal 2:

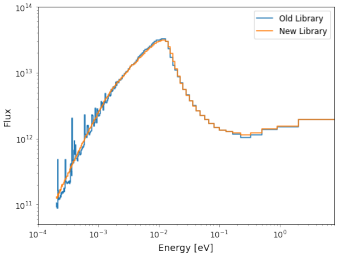
- Inelastic scattering in NCrystal is now based on scattering kernels
- For crystalline materials, scattering kernels can be generated on the fly from a DOS
- Other materials, like liquids, are supported through direct specification of a scattering kernel as tabulated S(q,ω) or S(α,β) values

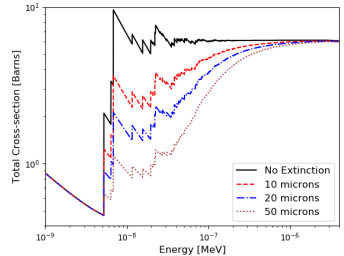


Groundwork III

Thermal scattering work at ESS:

- Processing of libraries using existing tools (NJOY)
- Improvement of neutronic codes (PHITS) to handle new libraries
- Inclusion of additional physics, such as extinction, into the creation of new libraries
- Generation of input for scattering kernels using path-integral molecular dynamics techniques





Thanks for your time.
Questions?