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PROGRAMME OF COORDINATED RESEARCH ACTIVITIES
Webpage: cra.iaea.org

PROPOSAL FOR RESEARCH AGREEMENT

PLEASE SEND YOUR PROPOSAL FOR RESEARCH AGREEMENT TO Official.Mail@iaea.org
ONLY DULY FILLED AND SIGNED PROPOSALS WILL BE PROCESSED.

1. CODE OF THE COORDINATED RESEARCH PROJECT (CRP) UNDER WHICH THE RESEARCH AGREEMENT SHOULD BE PLACED:
CRP F12026

2. TITLE OF THE COORDINATED RESEARCH PROJECT (CRP) UNDER WHICH THE RESEARCH AGREEMENT SHOULD BE PLACED:
Advanced moderators for intense cold neutron beams in materials research

3. TITLE OF THE PROPOSED RESEARCH AGREEMENT (should reflect the proposed research work):
Advanced models for liquid moderator cross sections

4. CONTRACTING INSTITUTION: **(The contracting institution can only be an institution with independent legal personality)***	**5. IMPLEMENTING INSTITUTION:** **(Where the research is performed) can be the contracting institution or a sub-institution, a branch of the main institution or a laboratory**
Inst. Name: Institut Laue-Langevin Street: 6, rue Jules Horowitz P.O. Box: 156 Postal Code: 38042 City : Grenoble Region/District : Country: France Tel.: +33 476 201 111 Fax: +33 476 483 906 Email: welcome@ill.fr Does the institution have an independent legal personality (*) ☒ Yes ☐ No	Inst. Name: Street: P.O. Box: Postal Code: City : Region/District : Country: Tel.: Fax: Email:

6. SUMMARY OF PROPOSED RESEARCH:
This project represents the ILL contribution to the CRP F12026. It focuses on the characterisation of materials used as neutron moderators (cross section), their modeling, and the understanding of microscopic behaviour through a more theoretical approach. As a result, we aim to contribute to the international neutron cross section data bases for water, *l*-D_2 and *l*-H_2, as well as other liquids such as methane, and mesytilene. This project fully fits in Action 1 of the CRP.

7. PROJECT PERSONNEL (if space provided below is insufficient, please attach additional sheets)

Chief Scientific Investigator (CSI)

Family Name :	First Name:	Gender: M/F	Date of birth yyyy-mm-dd:	Nationality:
FARHI	Emmanuel	M	1970-08-21	F

Telephone (office):	Fax (office):	Email (office):	Position held:
+33 476 207 135		farhi@ill.fr	Computer Scientist

Academic degree:	Subject:	Institution:	From:	To:
Ph. D	Quantum paraelectric anomaly study in KTaO3 perovskite	Montpellier II University, France	1995	1998
Eng.	Master Engineer Diploma	Ecole Supérieure de Physique et de Chimie Industrielles de la ville de Paris (E.S.P.C.I.), 10 rue Vauquelin, 75005 Paris, France.	1990	1994
M. Sc.	Laser-Matter interaction	Paris XI University, France (Orsay)	1993	1994

Related scientific experience: solid and liquid state physics, biology, neutron scattering, Brillouin light scattering molecular dynamics, optimisation, signal processing, Monte-Carlo simulation

Recent publications related to the project (within the past 2-3 years):

1. Dynamics of liquid Au from neutron Brillouin scattering and ab initio simulations: Analogies in the behavior of metallic and insulating liquids, E. Guarini, U. Bafile, F. Barocchi, A. De Francesco, E. Farhi, F. Formisano, A. Laloni, A. Orecchini, A. Polidori, M. Puglini, and F. Sacchetti , Phys. Rev. B 88 (2013) 104201.
2. Advanced sources and optical components for the McStas neutron scattering instrument simulation package E Farhi, C Monzat, R Arnerin, T Van Vuure, C Castán-Guerrero, C Hennane, P A Harraud, G Campioni, S Fuard, J Ollivier, P Willendrup Journal of Neutron Research 04/2013; 17(1).
3. Solid para-hydrogen as the paradigmatic quantum crystal: Three observables probed by ultrahigh-resolution neutron spectroscopy F. Fernandez-Alonso, C. Cabrillo, R. Fernández-Perea, F J. Bermejo, M. A. González, C. Mondelli, and E. Farhi, Phys. Rev. B 86, (2012) 144524.
4. Virtual experiments: Combining realistic neutron scattering instrument and sample simulations E. Farhi, V. Hugouvieux, M.R. Johnson, W. Kob, Journal of Computational Physics 228 (2009) 5251–5261.
5. iFit: A new data analysis framework. Applications for data reduction and optimization of neutron scattering instrument simulations with McStas, E. Farhi, Y. Debab, P. Willendrup , Journal of Neutron Research 04/2013; 17(1).

B. ***Secondary CSI (if applicable)***

Family Name :	First Name:	Gender: M/F	Date of birth: yyyy-mm-dd	Nationality:
CALZAVARA	Yoann	M	1975-04-20	F

Telephone (office):	Fax (office):	Email (office):	Position held:
+33 476 207 124		calzavara@ill.eu	Head of *Bureau Projet Calcul* service

Academic degree:	Subject:	Institution:	From:	To:
PhD	EXAFS on supercritical liquids	Université Joseph Fourier – St Martin d'Hères - FRANCE	1998	2001

Related scientific experience:

C. ***Main additional Scientific Staff***

Family Name :	**First Name:**	**Gender: M/F**	**Date of birth: yyyy-mm-dd**	**Nationality:**
GUARINI	Eleonora	F	1965-01-30	I

Telephone (office):	**Fax (office):**	**Email (office):**	**Position held:**
+33 457428146		guarini@ill.fr	Visiting scientist

Academic degree:	**Subject:**	**Institution:**	**From:**	**To:**
PhD	Two- and three-body interactions in fluid Kr by small angle neutron diffraction	University of Genova	1995	1998
Physics degree (laurea)	Neutron diffraction on liquid deuterium close to solidification	University of Firenze	1985	1994

Related scientific experience: liquid state physics, static and dynamic structure of liquids by neutron scattering, double differential cross section calculations for simple molecules, multiple scattering evaluation in neutron experiments, theoretical modeling of non-hydrodynamic liquids, development of big neutron instrumentation.

D. ***Main additional Scientific Staff***

Family Name :	**First Name:**	**Gender: M/F**	**Date of birth: yyyy-mm-dd**	**Nationality:**

Telephone (office):	**Fax (office):**	**Email (office):**	**Position held:**

Academic degree:	**Subject:**	**Institution:**	**From:**	**To:**

Related scientific experience:

8. PROPOSED RESEARCH PROJECT (if space provided below is insufficient, please attach additional sheets)

A. ***Description of Research Objectives and anticipated outcomes***

The aim of this project is to improve the accuracy of thermal and cold moderator cross-sections representation for materials such as water (light and heavy), liquid deuterium and hydrogen. We shall introduce experimentally measured dynamical structure factors $S(q,\omega)$ and convert them into an $S(\alpha,\beta)$ formalism. In parallel, molecular dynamics simulations for these liquids will complement these measurements, and semi-analytical models will be derived by fitting. Finally, new ACE will be made available for the community for these materials at different temperatures, as produced by e.g. NJOY/THERMR. We believe that such improved accuracy in the description of materials used as neutron moderators can lead to a better reactor physics modeling. Better description of these materials will also benefit to other neutron scattering ray-tracing simulation codes such as McStas and Vitess.

B. ***Scientific Scope of the Project (scientific problems to be addressed with overall and specific objectives)***

The accuracy of the international neutron cross section libraries could be tremendously

Improved by introducing measured dynamical structure factors S(q,ω). Indeed, recent studies based upon international benchmarks highlighted that the quality of the thermalization process treatment is fundamental for the validity of reactor physics calculations. Until now, the thermal neutron cross sections for reactor physics are usually ill described [6]. Indeed all of these evaluations are based upon experiments, like IR or Raman, which were performed with a momentum transfer q~0. The extension on the whole Q domain is carried out by approximate laws which become clearly wrong in the case of liquids like water, deuterium and hydrogen. Thus, even the accuracy of the most recent libraries is poor for the slowest neutrons.
Moreover, the present models used for these thermal cross sections undergo significant approximations for liquids like water or liquid hydrogen for example, even in the most recent libraries like JEFF3.1 or ENDF/B-VII.0.

C. ***Detailed Work Plan for the first year (including proposed methods or techniques)***
We shall focus on light and heavy water on the first year. We shall benefit from recent thermal neutron scattering experiments performed at the ILL on the IN4 and IN5 inelastic spectrometers. This data will be combined with molecular dynamics simulations and adjusted with semi-analytical models on a large dynamic range. The cross-section files for e.g. MCNP will be produced by applying the S(q,w) → S(a,b) Jacobian, then converting to ACE files. As a by product, new insight on both data and models for water will be achieved.

D. ***Detailed Work Plan for the second year (including proposed methods or techniques)***
As a second step, we shall focus on liquid deuterium, which is used as main cold neutron moderator at the ILL. Past experimental results, as well as potentially new experiments, will provide the starting data to compute the S(q,w) dynamic structure factor. In parallel, the possibility to use path integral Monte-Carlo for such quantum liquids (as classical potentials are not adapted) will be explored.

E. ***Detailed Work Plan for the third year (including proposed methods or techniques)***
Last, we shall consider the extension of the previous approach used for liquid deuterium to liquid hydrogen. Other moderators such as methane and mesitylene, also used as cold/warm moderators, could be envisaged.

F. ***Expected Outputs***
We aim to provide new neutron cross sections for water and cold liquid moderators. These cross sections will be usable with e.g. MCNP, GEANT4, McStas.

Please note that as a condition of an IAEA Research Agreement, all information, data and research results gathered during the course of the CRP are made freely available to other participants and other relevant authorized parties.

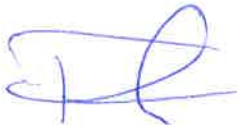
9. **PLEASE LIST FACILITIES (building, equipment - including type and name of manufacturer, and materials) PRESENTLY AVAILABLE WHICH WOULD BE USED FOR THE PROJECT**

Neutron scattering instruments (liquid diffractometer, time-of-flight inelastic spectrometer)
Computing facility (cluster)
Molecular dynamics codes (NAMD, VASP, ...)
Knowledge on liquid models
Neutron scattering instrument simulation (using McStas)
Reactor physics codes (MCNP)
Cross section data base tools (NJOY)
Data treatment tools including multidimensional fitting

10. PROPOSED COMMENCEMENT DATE: Jan 1st, 2014

11. SIGNATURES

CHIEF SCIENTIFIC INVESTIGATOR

FARHI		Nov 15th 2013
Name (in capitals)	Signature	Date

HEAD OF INSTITUTE

	HARRISON	15-11-13
Name (in capitals)	Signature	Date