

## Plan Overview

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*A Data Management Plan created using DMP Tool*

**DMP ID:** <https://doi.org/10.48321/D14DAE1B84>

**Title:** Determining Fundamental Properties of Tritiated Hydrogen to Advance Fusion Energy Technology

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**Project Administrator:** Timothy Prisk

**Funder:** United States Department of Energy (DOE) (energy.gov)

**Funding opportunity number:** DE-FOA-0003176

**Template:** Department of Energy (DOE): Generic

### **Project abstract:**

Deuterium-tritium mixtures are employed as thermonuclear fuel in inertial fusion energy. Elementary physical properties of the fuels, such as their density and thermal expansion, have never been measured. This gap in our knowledge is due to the practical and technical difficulties of carrying out experiments upon condensed tritium under cryogenic conditions. For this reason, the properties of tritiated fusion fuels are currently estimated by means of semi-empirical extrapolations from the corresponding properties of the non-radioactive hydrogens. Here, the author proposes a coordinated theoretical and experimental study of deuterium-tritium mixtures with the goal of accurately determining physical properties relevant to inertial fusion energy. In particular, the team will employ a combination of thermodynamic measurements, neutron scattering techniques, and ab initio quantum Monte Carlo simulations to characterize the deuterium-tritium fuel. The proposed research will provide key technical data for the optimization of inertial fusion energy implosions, thereby supporting the DOE goal of an economically viable fusion pilot plant.

**Last modified:** 07-08-2024

### **Copyright information:**

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## **Determining Fundamental Properties of Tritiated Hydrogen to Advance Fusion Energy Technology**

### **Data sharing and preservation**

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**Data management plans should describe whether and how data generated in the course of the proposed research will be [shared](#) and [preserved](#) and, at a minimum, describe how data sharing and preservation will enable [validation](#) of results, or how results could be validated if data are not shared or preserved.**

Research results will be published in peer-reviewed journals to ensure their wide dissemination among the scientific community. After publication, experimental data will be shared and preserved through the DOE Data Explorer, a public, web-based repository. Neutron scattering data obtained at the NIST Center for Neutron Research are made available eighteen months after their creation date via [ftp.ncnr.nist.gov](http://ftp.ncnr.nist.gov), in accordance with their data management plan. Code written for this project will be shared publicly on GitHub, an open-source software repository. All technical information and software produced over the course of the proposed research will be released through the LLNL Information Management process.

### **Data used in publications**

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**Data management plans should provide a plan for making all research data displayed in publications resulting from the proposed research open, machine-readable, and digitally accessible to the public at the time of publication. This includes data that are displayed in charts, figures, images, etc. In addition, the underlying digital research data used to generate the displayed data should be made as accessible as possible to the public in accordance with the [Principles](#) published in the DOE Policy for Digital Research Data Management. The published article should indicate how these data can be accessed.**

The subset of experimental and theoretical data published in graphical form will be included in the DOE Data Explorer repository created for this project.

### **Data management resources**

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**Data management plans should consult and reference available information about data management resources to be used in the course of the proposed research. In particular, DMPs that explicitly or implicitly commit data management resources at a facility beyond what is conventionally made available to approved users should be accompanied by written approval from that facility. In determining the resources available for data management at DOE Scientific User Facilities, researchers should consult the [published description of data management resources](#) and practices at that facility and reference it in the DMP.**

The raw data collected during the course of this research are not expected to exceed several gigabytes in size. Neutron scattering data obtained at NIST or ORNL are expected to fall within the normal data management resources provided by those institutions.

### **Confidentiality, security and rights**

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**Data management plans must protect confidentiality, personal privacy, [Personally Identifiable Information](#) and U.S. national, homeland, and economic security; recognize proprietary interests, business confidential information, and intellectual property rights; avoid significant negative impact on innovation and U.S. competitiveness; and otherwise be consistent with all applicable laws, regulations, agreement terms and conditions, and DOE orders and policies.**

The proposed research will not involve the collection of confidential information or Personally Identifiable Information. LLNL has established standards and policies regarding the transmission, storage, and destruction of data to protect U.S.

national interests, proprietary interests, and intellectual property rights. The Principal Investigator will conduct all work in accord with these requirements with support from LLNL's Office of Classification and Export Control, Industrial Partnerships Office, and Technical Information Department.

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## Planned Research Outputs

### Dataset - "Hydrogen Vapor Characterization"

Vapor pressure and mass spectroscopy measurements of non-radioactive hydrogen isotopologues and their mixtures.

### Dataset - "D-T Vapor Characterization"

Vapor pressure and mass spectroscopy measurements of liquid and solid D-T.

### Dataset - "Hydrogen-Deuterium mixture data set"

Neutron scattering and PIMC data from solid H<sub>2</sub>-D<sub>2</sub> mixtures of varying composition.

### Dataset - "Crystal structure of solid D-T"

Powder diffraction data and PIMC simulations of solid D-T.

### Software - "Path Integral Monte Carlo"

Extension of PIMC kernel to solid phase and the hydrogen isotopologues.

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## Planned research output details

| Title                               | Type     | Anticipated release date | Initial access level | Intended repository(ies) | Anticipated file size | License  | Metadata standard(s) | May contain sensitive data? | May contain PII? |
|-------------------------------------|----------|--------------------------|----------------------|--------------------------|-----------------------|--|----------------------|-----------------------------|------------------|
| Hydrogen Vapor Characterization     | Dataset  | 2029-12-30               | Open                 | DOE Data Explorer        |                       | Creative Commons Attribution 4.0 International | None specified       | No                          | No               |
| D-T Vapor Characterization          | Dataset  | 2029-12-30               | Open                 | DOE Data Explorer        |                       | Creative Commons Attribution 4.0 International | None specified       | No                          | No               |
| Hydrogen-Deuterium mixture data set | Dataset  | 2029-12-30               | Open                 | DOE Data Explorer        |                       | Creative Commons Attribution 4.0 International | None specified       | No                          | No               |
| Crystal structure of solid D-T      | Dataset  | 2029-12-30               | Open                 | DOE Data Explorer        |                       | Creative Commons Attribution 4.0 International | None specified       | No                          | No               |
| Path Integral Monte Carlo           | Software | 2029-12-30               | Open                 | GitHub                   |                       | Creative Commons Attribution 4.0 International | None specified       | No                          | No               |