INSPIRED: Inelastic Neutron Scattering Prediction for Instantaneous Results and Experimental Design

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Abstract

Inelastic neutron scattering (INS) has unique advantages in probing how atoms vibrate and how the vibrations propagate and interact. Such dynamic information is crucial in understanding various material properties, from heat capacity, thermal conductivity, phase transitions, and chemical reactions to more exotic quantum behavior. The analysis and interpretation of the INS spectra often start from a model structure of the sample, followed by a series of calculations to obtain the simulated spectra to compare with experiments. The conventional way to perform such calculations usually requires significant time, computing resources, and specialized expertise. Here, we present a new program named INSPIRED (Inelastic Neutron Scattering Prediction for Instantaneous Results and Experimental Design), which enables users to perform rapid INS simulations in several different ways on their personal computers in just a few clicks, with the crystal structure as the only input file. Specifically, the users can choose a pre-trained symmetry-aware neural network (coupled with an autoencoder) to predict the phonon density of states (DOS), 1D S(E) and 2D S(|Q|,E) spectra for any given structure. One can also choose an existing density functional theory (DFT) calculation from a database (containing over 12,000 crystals), and quickly obtain the simulated INS spectra for single crystals and powders. It is also possible to use pre-trained universal machine learning force fields to relax a given crystal structure, calculate the phonon dispersion and DOS, and, subsequently, the INS spectra. All these functions are implemented with a PyQt graphic user interface. We expect these new tools will benefit broad user communities

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and significantly improve the efficiency of experiment design, execution, and data analysis for INS.

Keywords: inelastic neutron scattering; spectroscopy; phonon; machine learning.

PROGRAM SUMMARY

Program Title: INSPIRED
CPC Library link to program files: (to be added by Technical Editor)
Developer's repository link: https://github.com/cyqjh/inspired (software)
Developer's repository link: https://doi.org/10.5281/zenodo.11478889 (database, models files, and virtual machine appliance file)
Code Ocean capsule: (to be added by Technical Editor)
Licensing provisions: MIT
Programming language: Python
Nature of problem: How to easily and quickly assess the expected INS spectra for a given crystal structure has been a major challenge in the INS user community. It is a main bottleneck affecting almost every stage of the workflow, from experimental design and steering to data analysis and interpretation. The widely used approach involving DFT calculations is time-consuming, requires advanced computing resources, and has a steep learning curve. With the growing power of neutron sources and more high-throughput INS experiments, there is a pressing need to address this problem, preferably by taking advantage of the recent developments in machine learning and artificial intelligence.
Solution method: We take a data-driven approach to tackle the problem. A symmetry-aware neural network is trained to make direct predictions from the crystal structure to either 1D spectra or latent space vectors, which can be decoded to reconstruct 2D spectra. The database used for the training contains over ten thousand crystals, which can also be used to calculate INS spectra for single crystals and powders. The recently emerging universal machine learning force fields provide another venue to accelerate the simulation significantly. All these solutions are implemented in a graphic user interface so that a user with no modeling/programming background or access to powerful computers can still easily run the workflow.

1. Introduction

Phonons are fundamental excitations of collective atomic vibration in condensed matter. Understanding phonons is one of the central themes in

condensed matter physics and materials science. A quantitative description of phonons is the basis for interpreting a material's properties. Inelastic neutron scattering (INS) is an indispensable tool for experimentally probing phonons and providing a comprehensive and quantitative description of them. In an INS experiment, a beam of neutrons is directed at a sample, and the energy and momentum changes between the incident neutrons and the scattered neutrons measure the phonons. Because the energy and momentum of thermal neutrons are comparable to those of phonons, INS has unique advantages in resolution, dynamical range, flexibility, and completeness. The high penetration power of neutrons also ensures the measured phonons reflect the bulk properties rather than those around the surface. In addition to phonons, INS is also a great tool to measure magnetic moments, thanks to the 1/2 spin of neutrons. However, the INS intensities from magnetic scattering are mixed with those from the phonons, making their separation a tricky task in some cases.

Despite these technological advantages, the interpretation and analysis of the INS spectra to convert the measured neutron scattering intensities into physical insight are often nontrivial. The most widely accepted approach involves atomistic modeling of a structural model, solving the interatomic interactions, often with density functional theory (DFT), and then calculating the lattice dynamics with density functional perturbation theory (DFPT) or the velocity autocorrelation from molecular dynamics, which are eventually converted to the simulated INS spectra corresponding to the experimental measurement. This workflow allows quantitative comparison between theory and experiment, which can further help us to modify the model, separate magnetic and nuclear scattering, revise a theory, improve an experimental plan, or discover a new phenomenon. Exciting as it is, the simulation process is often time-consuming, requires significant computing resources, and has a rather steep learning curve for researchers with no modeling background.

With the rapid development of computing hardware and advanced algorithms, including neural networks and deep learning, the data-driven approach is becoming increasingly appealing in addressing some of the most challenging computational bottlenecks. Large databases can now be generated with high-throughput computing, and complex neural networks can be trained as surrogate models to make rapid and accurate predictions. Many studies have followed this approach in the past few years to bring transformative changes to physics and materials research. This motivated us to develop easy, rapid, and user-friendly ways to obtain simulated INS spectra from

the structure. The program reported in this paper, INSPIRED, results from this endeavor. The following sections will briefly introduce the theoretical background, the program installation and interface, and some use cases.

2. Theory

The effort to create a database for the phonon density of states (DOS) started many years ago, and the progress has been well-documented in the literature (e.g., Ref [1]). Since phonon calculations, especially using DFT, are quite computationally expensive (a moderately complex system may take hours or even days on a computer cluster), the size of the available database is usually not very large. A prerequisite to using the database for data-driven predictions is efficiently representing the structure so that the atomic coordinates in a structural model can be directly connected with the phonon DOS. The recently developed Euclidean neural network is symmetry-aware, with equivariant to 3D translations, rotations, and inversion intrinsically built into the network's architecture [2, 3]. This dramatically improved the data efficiency, compared to the conventional encoding, which includes a large fraction of redundant information. Using an optimized Euclidean neural network, Chen et al. successfully achieved direct prediction of phonon DOS from the crystal structure [4]. However, more barriers must be overcome to take a step further and predict INS spectra directly. First, to obtain an INS spectra database for training, one must perform a high-throughput INS simulation on an existing phonon database. Several programs developed in recent years are available, such as OCLIMAX [5], AbINS [6], and Euphonic [7]. In this work, we use OCLIMAX as the INS calculation engine. Moreover, for INS simulations, one needs not only phonon DOS, but also the force constants to obtain the eigen-energy and engien-mode at any given q in the Brillouin zone. Most published phonon databases do not have such information. The phonondb@kyoto-u by A. Togo included the DFT calculated forces for over 10,000 crystals [8]. The OCLIMAX program and the phonondb@kyoto-u database were used to publish the first large-scale synthetic INS database [9]. Second, unlike the 1D phonon DOS, the INS spectra can be in 2D or high dimensions. For example, the powder 2D S(|Q|,E) with the most common E and Q binning can result in ∼100,000 pixels, which is too high for the current neural network to predict directly. Cheng et al. employed an autoencoder to significantly compress the data in the 2D S(|Q|,E) into a 50-dimension latent space so that all we need to do is to connect the crystal

structure with the latent space representation of the 2D spectra, and then using the decoder to reconstruct the 2D spectra from the latent space vector [10]. This approach has succeeded in performing straightforward and rapid predictions for complex structural models that are, at best, difficult and often infeasible using conventional DFT calculations. One major advantage is that the users can submit any structural model, small or large, ordered or disordered, and it will always return the result within seconds. The users can be reasonably confident about the overall profile of the predicted spectra, given that the training database included nearly 100 elements in the periodic table and the mean squared errors in the testing dataset were satisfactory.

Although the neural network model can be extremely helpful in experimental design and preliminary data analysis, there are certain limitations. First, INS spectra vary with instrument geometry and configuration, even for the same material. The current INS database was compiled for certain representative configurations; therefore, the trained neural network can only make predictions for these configurations. Second, all current predictions are for powder samples. Single crystal INS prediction for any crystal is not available yet, and it will likely be much more challenging to implement. Third, without the force constants, there is an overall lack of flexibility in examining the details and performing accurate quantitative analysis and interpretation. For these reasons, the direct prediction approach should be complemented with methods for a more comprehensive solution. One alternative possibility is that if the crystal structure of interest is already in the database, one can perform INS simulations within a relatively short time, usually within minutes. This is not as fast as direct prediction but provides flexibility in calculating the spectra for any instrument configuration and single crystal. Of course, this is only limited to the crystals already in the database. What if we would like to do the same for a different crystal? An important advance in the past few years is the development of machine learning force fields (MLFFs) based on DFT-calculated forces. These force fields can be accurate at close to DFT-level, yet they are much faster to compute compared to DFT. The MLFFs were originally trained and used for a specific composition/system, but very recently, large foundation models have been trained to obtain "universal" MLFFs that can cover the most common elements in the periodic table, such as the work by Batatia et al. [11, 12, 13], Deng et al. [14], Chen et al. [15], Merchant et al. [16], and Choudhary et al. [17] In principle, the availability of such universal MLFFs makes it possible to perform fast structural relaxation, phonon calculation, and INS

simulation for any given crystal with both speed and flexibility. This is an enormous achievement; statistically, the performance is very good. However, one note of caution is that for a specific case, the phonon calculations using the universal MLFFs are not always satisfactory – large discrepancies with DFT and instability are sometimes possible. This is not surprising given the great challenges of this undertaking, from the size of the training data to the complexity of the neural network. We are optimistic that the quality of the universal MLFFs will continue to improve, and they will play an increasingly important role in INS modeling and analysis.

3. About INSPIRED

Inspired by the above development in databases and deep learning models, we have developed the INSPIRED program to provide a user-friendly interface so the neutron scattering community can benefit from these recent advances. The graphic user interface (GUI) was built with PyQt. The program was written in Python to implement three key functions. First, it can perform direct prediction of phonon DOS (including partial DOS), 1D S(E) spectra for the indirect geometry spectrometers (VISION/TOSCA[18, 19]), and 2D powder S(|Q|,E) as measured by direct geometry spectrometers (e.g., the ones at the Spallation Neutron Source [20]) from any given structure. Second, it can calculate the INS spectra for powders and single crystals for any crystal found in the database. Third, it can perform structural optimization, phonon calculation, and INS simulation for powders and single crystals for any given crystal, using a universal MLFF of the user's choice (MACE[11, 12, 13], CHGNet[14], and M3GNet[15]). In all cases, we implemented different ways to visualize the spectra, including an interactive 2D cross-section plot for the 2D spectra. Building upon previous developments in DFT database and machine learning models, we focused our current work on user-friendly implementation that helps translate technological progress to tangible tools that will benefit general neutron-scattering users. The high-level workflow illustrating the three routes in INSPIRED is shown in Figure 1.

4. Installation of the program

The software is freely available on GitHub [21]. The database and pre-trained neural network models can be downloaded at Zenodo [22]. The pro-

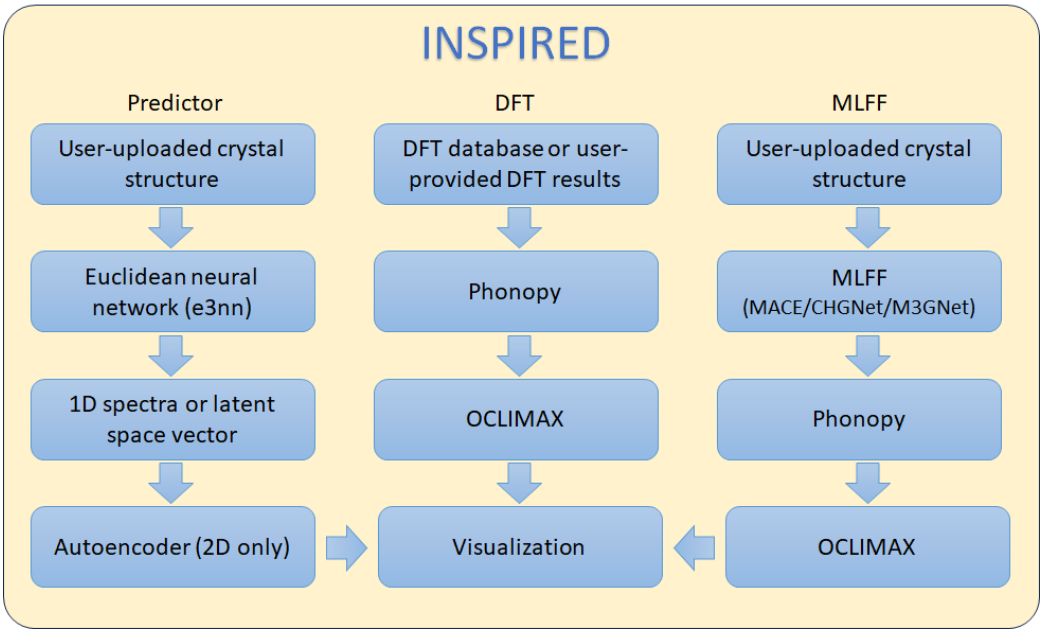

Figure 1: An illustration of INSPIRED workflow showing its main components.

gram requires a Linux operating system and a conda environment. The following are the high-level installation steps.

1. Install Anaconda or Miniconda for Linux [23].

2. Download the software from GitHub. Follow the instructions in the README.md file to create, install, and activate the required conda environment.

3. Download and unzip the database (dftdb.tar.gz) and pre-trained neural network models (model.tar.gz) from Zenodo.

4. Create a working directory where you would like to save all your output files. Go to this directory and run "inspired".

If you do not have a Linux computer or cannot install the software properly, we also provide a pre-installed Linux virtual machine (VM). The VM appliance file (inspired_vm.ova) can also be downloaded at Zenodo [22]. Then, you can install VirtualBox [24] on your computer (e.g., Windows or MacOS) and import the VM appliance. After starting the VM, you can simply open a terminal in the VM and run "inspired". More details can be found in the README.md file on GitHub.

When using INSPIRED, it is important to ensure the "Current Working

Directory" (CWD) is correctly set, as this is where the program creates/reads all its input and output files. The default CWD is where you started INSPIRED, and once this program is running, you can change it in the Menu. It is strongly recommended that a new folder be created for each material to avoid mixed input/output files and potential errors.

5. Use case: direct prediction

The first thing we can do with INSPIRED is to make instantaneous predictions of phonon DOS and INS spectra from any given crystal structure using the "Predictor" tab. The user can upload a structure file in CIF format or the VASP [25] POSCAR/CONTCAR format, choose the type of spectra to predict, and get the results in seconds. Apart from direct visualization of the results in the GUI, the numeric data files of the spectra will be saved in the CWD with a timestamp in the file names. It should be noted that fractional occupancies, sometimes present in CIF files, are currently not supported. The fractional occupancies do not represent a physically meaningful local structure; they represent a statistical description of a crystal structure with structural/compositional disorder. A common way to convert the statistical picture to a realistic structural model is to create a supercell (i.e., multiple repetitions of the unit cell in space) and fill the fractionally occupied sites according to the probability and other physical constraints (e.g., fragmented or heavily distorted molecules are not allowed, and two atoms cannot be too close to each other). Once the user obtains the supercell, it can be uploaded for prediction. Unlike DFT calculations, which slow down dramatically with the increasing size of the cell (and eventually become unfeasible), the predictions performed here are not sensitive to the system size. It can easily handle thousands of atoms without any issues. Figure 2 shows an example of using INSPIRED to predict and visualize various spectra for $Ba_3ZnRu_2O_9$. The corresponding experimental spectra can be found in Ref [10].

6. Use case: DFT database

The second function of INSPIRED, which comes naturally with the availability of the DFT database, is to make quick calculations of the INS spectra using the DFT force constants. This function is only available for a crystal that is already in the database. The DFT phonon database contains 10,023

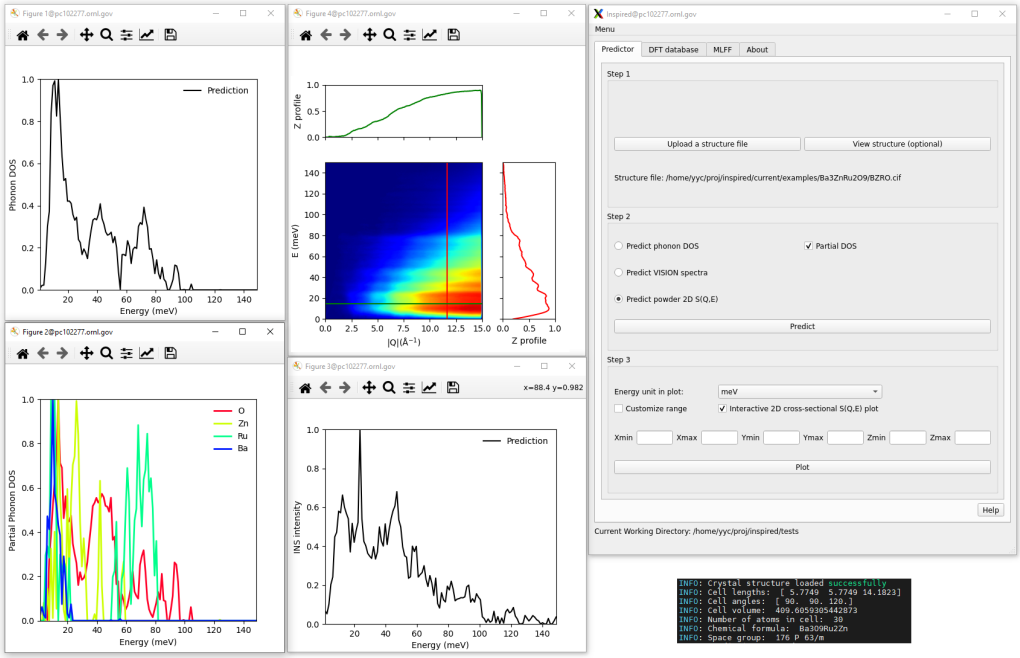

Figure 2: Screenshots of the "Predictor" tab and some prediction results. The left panels show the predicted total and partial phonon DOS, the VISION/TOSCA 1D S(E) spectrum, and the 2D S(|Q|,E) in an interactive cross-section plot. The right panels show the GUI (top), and the text output in the terminal shows the basic crystal information (bottom).

entries from the phonondb@kyoto-u database [8] and about 2700 additional entries from the current authors (more will be available in future release), all of which are based on crystals from the Materials Project [26]. On the "DFT database" tab (Figure 3), the users can search a crystal by different categories (composition, materials ID, space group, etc.) If the crystal of interest is found, the users can check the phonon dispersion and DOS quickly before proceeding to the INS simulation. The phonon and INS simulations using Phonopy [27] and OCLIMAX can be set up in the pop-up window, where one can choose to use the default settings, load an existing params file, or make manual changes. Note that the way single crystal simulation is set up (in the right column) is new in INSPIRED and unavailable in the previously released standalone OCLIMAX. Detailed instructions can be found by clicking the "help" button. Once all parameters are finalized, the users can save them in a (different) params file and close the pop-up window. The next step is to run the INS simulation, which usually takes seconds to minutes, depending on the size of the system and the complexity of the simulation. Progress can be monitored in the terminal window, and the run can be terminated if necessary. Figure 4 shows a few examples of the simulated INS for single crystal Cu. The corresponding experimental spectra can be found in Ref [28]. Note that the xyz ranges can be customized when making these plots. The energy unit used in the plots can also be changed.

7. Use case: universal MLFFs

The third feature of INSPIRED takes a different approach to utilizing machine learning for accelerated phonon and INS simulations. The recently developed and published universal MLFFs have shown great promise in modeling atomic structure and dynamics with much faster speed, unprecedented transferability, and satisfactory accuracy. We thus implemented a workflow in INSPIRED, on the "MLFF" tab, to perform phonon and INS simulations from scratch, using one of the universal MLFFs (MACE [11], CHGNet [14], M3GNet [15]). This is very similar to the conventional workflow, and the only difference is that, instead of using DFT for structural optimization and phonon calculation, the much faster surrogate MLFFs are used here. This can accelerate the process by orders of magnitude (minutes vs hours/days), and it also eliminates the need for powerful computers or the know-how to run a DFT calculation. Our tests indicate that for many systems, the simulated INS spectra using the MLFFs are satisfactory. However, there are also cases

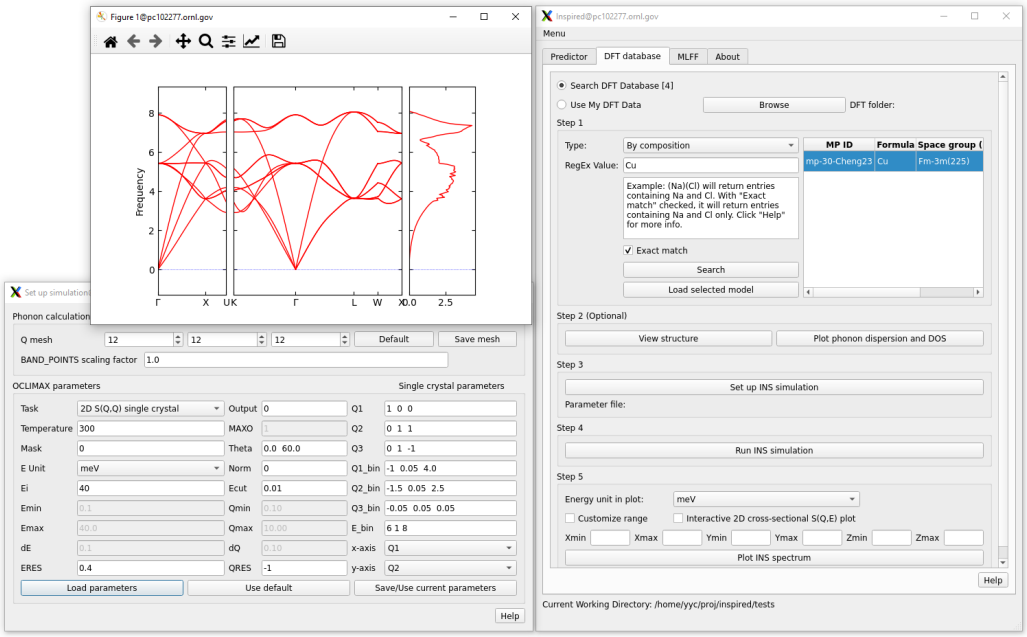

Figure 3: Screenshots of the "DFT database" tab (right), the OCLIMAX setup interface (left bottom), and the phonon dispersion and DOS of the selected crystal (left top).

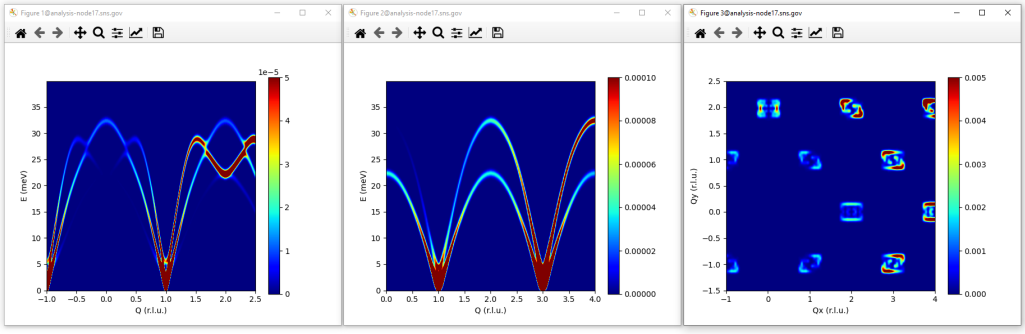

Figure 4: Simulated INS spectra of single crystal Cu. (Left) S($\mathbf{Q}$,E) along [H,1,1] (Middle) S($\mathbf{Q}$,E) along [1,K,K] (Right) $S_E(\mathbf{Q_x},\mathbf{Q_y})$ with $\mathbf{Q_x}$=[H,0,0], $\mathbf{Q_y}$=[0,K,K] and energy integrated in 7-9 meV.

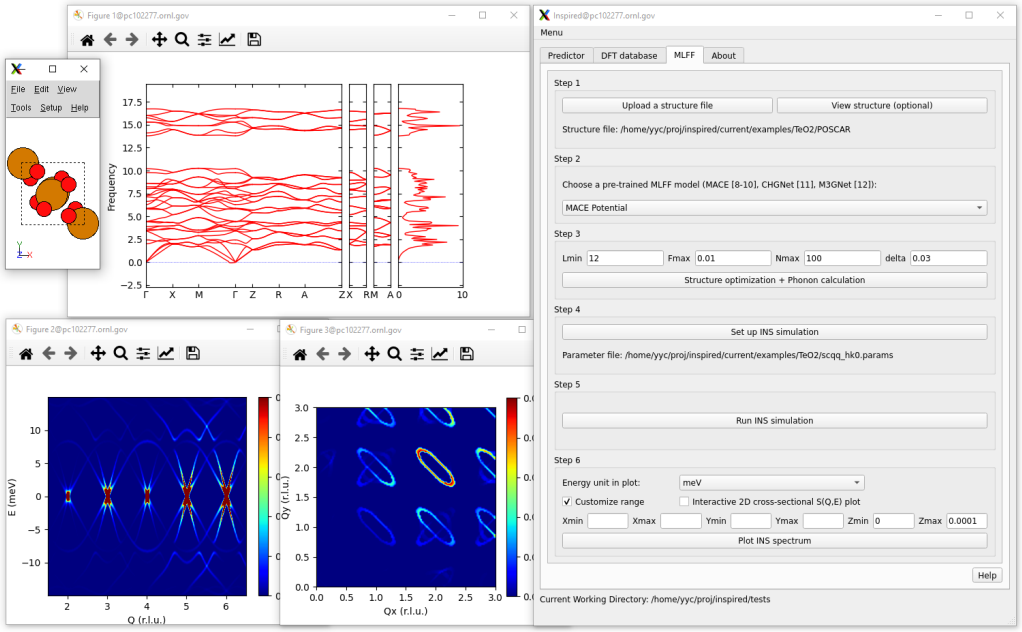

Figure 5: Screenshots of the "MLFF" tab (right). The calculated phonon dispersion and DOS are shown in the left top panel (with a view of the crystal structure), and the simulated single crystal INS spectra are shown in the left bottom panels, for S($\mathbf{Q}$,E) along [1,0,L], as well as $S_E(\mathbf{Q_x},\mathbf{Q_y})$ with $\mathbf{Q_x}$=[H,0,0], $\mathbf{Q_y}$=[-1,K,0], and energy integrated within 3.5-4.5 meV.

where the calculated phonons are unstable or significantly softer/harder than they should be. Users are advised to carefully examine the calculated phonon dispersion and DOS before proceeding to the INS simulation and data interpretation. Figure 5 illustrates an example using TeO_2. The corresponding experimental results can be found in Ref [29].

8. Summary

Obtaining the expected INS spectra from a given structure has been a major bottleneck in the data pipeline for INS experiments. The conventional approach requires significant computing resources, special expertise, considerable human effort, and long calculation time. Recent advances in high-throughput INS simulations and machine learning for materials sciences have set the stage for addressing this long-standing issue. The INSPIRED program is developed as a user-friendly interface for researchers to perform

easy and quick phonon and INS predictions, simulations, and visualization, with state-of-the-art algorithms as the engines. The users do not need modeling expertise or access to powerful computers. The results can be obtained from a structure file and a few clicks. INSPIRED can handle more complex systems than what we can currently afford with DFT, and the running time on a personal computer usually ranges from seconds to minutes. It is expected to be a useful tool for the INS user community.

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