Abstract
Neutron scattering provides a sensitive probe for materials structure and dynamics and has had a profound impact on research ranging from quantum topological materials to archaeology to aerospace alloys. These experiments are incredibly data-rich and often challenging to interpret. Computational studies have been integral in the growing success of neutron science. From data collection and reduction to analysis and interpretation, computers are used at every stage of modern neutron experiments. State-of-the-art software allows for a deeper understanding of these powerful unique experiments. This themed issue, guest-edited by Dr. Jeff Armstrong, Dr. Keith T Butler, and Dr. Matthew R Ryder, brings together a collection of research highlighting the state-of-the-art in the application of computers in neutron science.

Editorial
Neutron spectroscopy is one of the few tools that provide a full characterization of the atomistic dynamics of materials across a wide length and time scale. The information content of each spectrum, however, is dense, and analysis through simple analytic models is severely limiting. To extract the full information content, the use of computer simulation is essential for most complex systems. We open this collection with an initial review of how computation and experiment have worked together in neutron spectroscopy to provide essential advances in understanding the dynamical properties of materials [1]. We then present a range of research articles that highlight how computers and neutrons are being used to explore a diverse range of systems and some of the latest developments in software for neutron science.

The extra information that neutron spectroscopy provides when compared to the likes of infrared and Raman is exemplified in a study of an iridium metal complex by Parker [2]. In this study, all three spectroscopic techniques are employed on two polymorphs of the complex. A shortcoming of Raman spectroscopy becomes apparent since a direct comparison between theory and experiment is not shown, due to the high computational cost. The necessity for inelastic neutron scattering (INS) is evident, as the high-frequency modes for both polymorphs appear equivalent, and only INS can draw a direct comparison between experiment and theory for the intermolecular modes which are sensitive to the crystal morphology.

A primary strength of coupled density functional theory-lattice dynamics (DFT-LD) and neutron spectroscopy is the ability to decompose in silico spectra on a molecule-by-molecule basis. This is demonstrated in the article by Mukhopadhyay [3], where a study of hydrogen bonding in organic ferroelectrics was able to distinguish between intramolecular hydrogen bonding, intermolecular hydrogen bonding, and non-hydrogen-bonded protons, and subsequently attribute the ferroelectric nature to that of the intermolecular hydrogen bonding. The article also highlights an important technical point on the necessity of including dispersion corrections for such organic molecular crystals. Without these corrections for such organic crystals, the experimental crystal structure is often not accurately reproduced during the energy minimization phase, and as a consequence, the resultant vibrational density of states does not match that of the experiment.
This theme of the importance of the quantitative accuracy of computational models across a wide range of frequencies is further highlighted in the next article [4], which employs the technique of deep inelastic neutron scattering (DINS). DINS is analogous to Compton scattering, where the instantaneous momentum of each atomic species is sampled and can be quantified by the width of the resultant peak. This instantaneous momentum has contributions from all motions of the system, and the sensitivity to the peak width of this technique is high. The degree of precision obtainable by DFT-LD calculations is demonstrated for an oxyhydride, where comparisons across a wide temperature range displays excellent agreement with the DINS measurement. This combination of DINS and ab initio calculation was also shown to play a critical role in uncovering isotopic effects for the nuclear quantum dynamics of isopropyl molecules in the condensed phase [5]. This work then links into muoniated isopropyl, being the first time that DINS has been used to gain knowledge of the nuclear and spin dynamics of Mu.

The use of computational techniques is by no means limited to dynamics/spectroscopy, but is, of course, essential in the determination of structure as demonstrated in the contribution from Cai and coworkers [6]. Reverse Monte Carlo methods were, in fact, some of the first computational models applied to neutron data, aiding in our understanding of disordered materials. In this study, a combination of diffraction and total scattering measurements is used to understand the orientational disorder and phase transitions in potassium cyanide as well as providing information about the instantaneous strain. Importantly the article serves as a pedagogical case for a new theoretical methodology. This methodology employs a high order expansion of the bond orientation distribution function in terms of symmetry-adapted orientational functions, alleviating a common problem for diffraction studies of maintaining positive definiteness.

Wang and coworkers investigated the effects of interchain and intrachain association in determining the static structures of polymers in the melt state using a combined approach of small-angle neutron scattering (SANS) and molecular dynamics (MD) simulations [7]. Their results suggested that while interchain interactions dominate in the melt state of the polymer systems, the structures can be strongly influenced by the presence of intrachain loops. Therefore, to fully understand the dynamics and viscoelastic properties, the presence of such loops should be taken into consideration when studying associative polymer networks.

Using Brownian dynamics simulations, Sánchez-Díaz, Chen, and coworkers reported a connection between the shear-induced microstructural distortion and nonlinear rheology of concentrated colloidal suspensions [8]. They reported a non-uniform flow in the nonlinear shear-thinning regime resulting from a localized elastic response, which they define as the transient elastic zone (TEZ) at mesoscopic length scales. However, the body of colloids under shear behaves like a fluid at longer length scales. Nevertheless, they report that the short-lived TEZ plays an essential role in determining the observed rheological behavior, which could be relevant to a wide variety of highly interacting soft matter materials.

The first comparison of all-atom and coarse-grained molecular dynamics approaches to assess the reliability of the techniques for the analysis of neutron reflectometry measurements is reported by McCluskey, Edler, and coworkers [9]. They use three potential models, namely the all-atom Slipid, united-atom Berger, and coarse-grained MARTINI models, and benchmark them against a traditional layer structure analysis method to determine the minimum simulation resolution required to reproduce the reflectometry results accurately. They report that Berger and Slipid potential models are in reasonable agreement with the experiment, but that the best results are obtained from the traditional monolayer model because of the added structural flexibility. However, they use the insight obtained from the Slipid potential results to improve the traditional approach and obtain an optimized model lipid monolayer.

Software is essential across the lifetime of a neutron experiment. From the design of the instrument, to the collection and analysis of data from the experiment. The software packages highlighted in this collection demonstrate the pivotal role that codes developed at neutron facilities are playing in driving the next generation of neutron science.

Lin and coworkers present the latest updates of the MCVINE package [10]. The authors present the latest updates in the software as well as highlighting the immense utility of software for the design of everything from new neutron instruments at the second target station of the SNS at Oak Ridge to novel sample holder environments. The NEUIT package, also developed at Oak Ridge allows for simulations to applied for preparation of samples and feasibility estimates; critical when preparing samples for neutron imaging studies [11]. The availability of the software can save considerable amounts of experimental time and frustration by allowing virtual testing of new ideas.

The increasing availability of new and more powerful neutron experiments means that there is an ever-increasing volume of data that needs to be processed. Again, new software packages are appealing to meet these demands. BEAN (Bragg Edge Analysis) is a code developed at the ISIS neutron and muon facility to meet the increased demand as a result of new technical capabilities at the IMAT beamline [12]. The BEAN software developed by Liptak and coworkers allows for semi-automated analysis of Bragg edge transmission. The code combines Python and Qt to provide a user interface and also includes standard tools used in the analysis of Bragg
edges, such as principal component analysis. The MIEZEPY software developed between the Julich Centre for Neutron Science, the Heinz Maier-Leibnitz Zentrum and the Technical University Munich facilitates the analysis of increasingly complex 4D datasets arising from Modulation of intensity with zero effort (MIEZE) neutron experiments [13]. These experiments are implemented at a number of neutron sources, including MLZ, J-Parc, and ISIS.

Bilheux and coworkers provide an overview of existing approaches to neutron imaging analysis, ranging from pure code-based tools to interactive GUIs [14]. The authors present the pros and cons of the various approaches and make a compelling case for the use of Jupyter notebooks as a happy medium, meeting the requirements of the scientific population. Jupyter notebooks allow for the implementation of flexible code workflows, with minimal coding experience. Additionally, the advent of cloud-based services such as Jupyter Hub means that the heavy lifting of the computation can be performed remotely without the need for the end-user to install bespoke software or environments.

A recurring theme throughout the new software presented in this edition is the embracing of the standards of software engineering by the neutron science community. The Research Software Engineer initiative has been gaining increasing recognition; the importance not just of software but of high-quality, stable, reusable, and reproducible software has become a central requirement across the sciences increasingly. It is heartening to see so many of the packages presented here, adhering to the principles of this movement. For example, the MIEZEPY package follows software engineering patterns when developing the interface to ensure maximum stability and extensibility [13]. Many of the packages are also distributed via public repositories and come with open source licenses. This concerted move towards high-quality, open code is immensely encouraging for the future of software in neutron science.

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