



Technical University of Denmark



## Ph.D scholarship in “Magnon-phonon coupling in FePS<sub>3</sub>”

*This is a joint programme between the Institut Laue-Langevin (ILL) and the Technical University of Denmark (DTU). The project combines advanced condensed matter computation and state-of-the-art neutron scattering experiments to study the interplay between magnetic and crystal lattice vibrations in layered van der Waals compounds.*

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The PhD provides a unique opportunity to engage into cutting edge research on magnetism in two-dimensional materials using *both* first principles theoretical methods and neutron scattering techniques. The position will give you an ideal starting point for a career in academia and you will acquire advanced skills in computational solid state physics and in state-of-the-art neutron scattering methods. You be formally affiliated with both institutions but will be employed at ILL and enrolled at DTU.

The topic of the project is the intricate interplay between magnons and phonons in the layered van der Waals compound FePS<sub>3</sub>. These types of compounds are currently highly researched as they may be delaminated down to one atomic layer, similar to graphene. FePS<sub>3</sub> is particularly interesting as it is intrinsically magnetic, offering great insight into the fundamental magnetism in low dimensions and having potential for applications in graphene-based technology. The compound is also highly magnetostrictive, with a strong coupling between the magnetic and crystal structures. The key to understanding of the properties of the compound lies in the crystal lattice vibrations, known as phonons, the magnetic excitations, known as magnons, and in particular the interaction between them. Such interactions are currently poorly understood in condensed matter physics. Studying them in FePS<sub>3</sub> will lead to the understanding of its physical properties, and will serve as a basis for a better comprehension of magneto-lattice coupling.

You will study magnon-phonon interactions in FePS<sub>3</sub> by means of inelastic neutron scattering experiments guided by first principles computational modelling. After a short integration period in France, some time towards the beginning of the project (six months) will be spent at DTU focusing on learning and applying density functional theory for the analysis of magnon-phonon spectra. The remaining time (2.5 years) will be spent at ILL performing and analysing neutron scattering experiments, which will be continuously supported by first principles simulations. There will thus be a strong interplay between experiments and theory throughout the entirety of the project period.

The project combines the resources of two leading institutions. DTU is a leading technical university globally recognized for the excellence of its research, education, innovation and scientific advice. The ILL is an international research centre at the leading edge of neutron science and technology, operating a neutron source with exceptionally high neutron flux and around 40 cutting-edge instruments. You will be a part of a vibrant and cohesive cohort of students from across Europe with regular social and development events, and experience life in a cosmopolitan city at the foot of the French Alps. This project will allow you to build your research direction and establish a network of contacts and collaborators across Europe and is an excellent springboard into a career in magnetism and neutron scattering, or beyond.

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