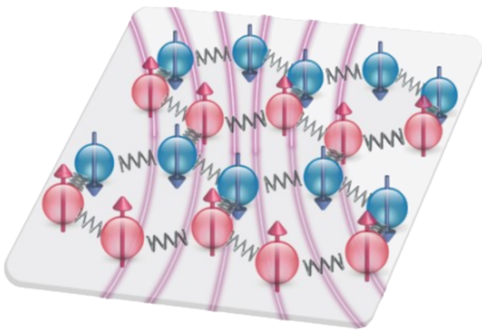
In Silico Characterization of Magnon–Phonon Coupling in Two-Dimensional Magnetic Materials

Two-dimensional (2D) magnetic materials, such as monolayer chromium trihalides and manganese dichalcogenides, have recently drawn immense attention of both theoretical and experimental research, with many exciting emerging properties and significant potential for applications, ranging from low-power spintronics to quantum computing [1]. The use of magnetic (spin) degrees of freedom, and the low-energy collective magnetic excitations (spin-waves, magnons) as the information carrier is a direction chosen for devices intended to replace CMOS technology, towards fast yet energy-efficient platforms for information processing [2]. Combining this with the strong tunability of magnonic behavior in 2D materials [3] and the fact that high-frequency magnon modes have been readily detected in such systems [4-6], one can promote 2D magnonics to the prime echelon of candidates for cutting-edge spintronic applications. Nonetheless, the propagation of magnetic excitations in realistic materials is accompanied by the combination of several physical phenomena which can significantly affect the transmitted magnonic signals, for example, the interaction with the material phonons (mechanical vibrations in the atomic structure). The interaction between magnons and phonons allows hybridization between magnetic and phononic resonances, which provides possible mechanisms to excite, manipulate, and detect magnons by coupling to phononic modes. In fact, magnon and phonon modes have been shown to share similar wavenumbers in atomically-thin chromium tri-iodide [6], and a strong coupling between the magnon band and its adjacent phonon mode has been directly observed via magneto-Raman spectroscopy in the antiferromagnetic monolayer $FePS_3$ [5]. Despite the recent observations, a complete understanding of magnon–phonon coupling in 2D magnetic materials is missing, and the physics of such phenomena mostly unnexplored. Therefore, in this project we will calculate the interaction of phonons and magnons in selected 2D materials by combining *ab initio* calculations of magnetic parameters in the presence of different phonon modes and spin-dynamics simulations of spin-wave propagation, in order to fully characterize the effects of magnon–phonon coupling to the spin-wave dispersion in such 2D materials.



References

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