

Computational study of changes of exchange interactions in the vicinity of the surface

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Magnonics is an emerging field that could transform information storage and processing. It promises lower costs than conventional electronics and much higher operating speeds—potentially up to the THz regime. Achieving these advances requires understanding the phenomena governing magnon behavior. As highlighted in the "2021 Magnonic Roadmap" review article [1], a major challenge is the direct imaging of magnons at high spatial resolution. Solving this would accelerate research and the development of advanced magnonic devices.

It has been suggested that monochromated scanning transmission electron microscopes could be suitable for this task [2,3]. This technique enables nanoscale studies, allowing researchers to observe local changes in magnetic interactions and investigate how magnon dispersion varies near interfaces.

In our work, we combined density functional theory with atomistic spin-dynamics to understand how interfaces influence magnon dispersion—a key factor for designing nanostructures in modern applications.

We studied body-centred cubic iron (Fe) and its ultrathin layer in a vacuum to see how broken symmetry affects exchange interactions and magnon behavior. Magnetic exchange integrals were calculated using SIESTA, and we assessed interactions between non-equivalent atoms based on their distance from the bcc Fe-vacuum interface. We also used UppASD for atomistic spin-dynamics simulations to explore local magnetic dispersions. Snapshots of magnetic structures from these calculations served as input for inelastic electron scattering simulations.

References:

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