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Solid State NMR Spectroscopy with Quantum Espresso

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Recent advances in the application of *first principles* calculations of NMR parameters to periodic systems [1] and the steady increase of computational power, have become attactrove in their use to support experimental measurement. Such calculations often play an important role in the emerging field of *NMR crystallography*, where NMR spectroscopy is combined with techniques such as diffraction, to aid structure determination [2]. In this talk I will introduce the capabilities of QE-GIPAW [3], which is based on the popular DFT package Quantum Espresso [4]. After reviewing the underlying theory of the magnetic response of periodic systems, I will highlight how QE and QE-GIPAW can be used in a computational workflow, integrated with NMR/EPR simulation software like Simpson [5] and EasySpin [6]. I will present two case studies of the structure determination of purely inorganic and pharmaceutical crystal polymorphs, where the QE-GIPAW provided a correct assignement of the ^{1H} and ¹³C NMR shifts.
Finally, I will briefly illustrate the plans to provide a user friendly *cif-to-spectrum* workflow to be run in the cloud or on premises, thus avoiding the complication of installing and compiling the complete software stack.

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