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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 attractive 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 assignment of the ^1H and ^{13}C 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.

[1] C. J. Pickard and F. Mauri, All-electron magnetic response with pseudopotentials: NMR chemical shifts, *Phys. Rev. B* 63, 245101 (2001); J. R. Yates, C. J. Pickard and F. Mauri, Calculation of NMR chemical shifts for extended systems using ultrasoft pseudopotentials, *Phys. Rev. B* 76, 024401 (2007)

[2] S. E. Ashbrook and D. McKay, Combining solid-state NMR spectroscopy with first-principles calculations – a guide to NMR crystallography, *Chem. Commun.* 52, 7186 (2016); D. L. Bryce, NMR crystallography: structure and properties of materials from solid-state nuclear magnetic resonance observables, *IUCrJ* 4, 350 (2017)

[3] N. Varini, D. Ceresoli, L. Martin-Samos, I. Girotto and C. Cavazzoni, Enhancement of DFT-calculations at petascale: Nuclear Magnetic Resonance, Hybrid Density Functional Theory and Car-Parrinello calculations, *Comp. Phys. Commun.* 184, 1827 (2013); <https://github.com/dceresoli/qe-gipaw>

[4] P. Giannozzi et al., QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials, *J. Phys.: Cond. Mat.* 21, 395502 (2009)

[5] M. Bak, J. T. Rasmussen and N. C. Nielsen, SIMPSON: A General Simulation Program for Solid-State NMR Spectroscopy, *J. Magn. Res.* 147, 296 (2000)

[6] S. Stoll and A. Schweiger, EasySpin, a comprehensive software package for spectral simulation and analysis in EPR, *J. Magn. Res.* 178, 42 (2006)

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