NMR and EPR parameters from ab-inito

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Abstract: Nuclear Magnetic Resonance (NMR) and Electron Paramagnetic Resonance (EPR) spectroscopy are powerful tools for studying the structural and electronic properties of liquids and solids. NMR and EPR parameters can be calculated routinely by several ab-initio codes both molecular and periodic. In this talk I will present the QE-GIPAW code which uses plane waves and pseudopotentials, and is particularly suited to calculate solid-state NMR and EPR parameters. As an application of both, I will present the calculation of paramagnetic-NMR shift in olivine-type $LiTMPO_4$ (TM = Mn, Fe, Co, Ni).