Abstract Submitted
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Determination of NMR chemical shifts for cholesterol crystals from first-principles EMINE KUCUKBENLI, STEFANO DE GIRONCOLI, International School for Advanced Studies (SISSA) and CNR-IOM DEMOCRITOS Simulation Center, via Bonomea 265, 34136 Trieste, Italy — Solid State Nuclear Magnetic Resonance (NMR) is a powerful tool in crystallography when combined with theoretical predictions. So far, empirical calculations of spectra have been employed for an unambiguous identification. However, many complex systems are outside the scope of these methods. Our implementation of ultrasoft and projector augmented wave pseudopotentials within *ab initio* gauge including projector augmented plane wave (GIPAW) method in Quantum Espresso simulation package allows affordable calculations of NMR spectra for systems of thousands of electrons. We report here the first *ab initio* determination of NMR spectra for several crystal structures of cholesterol. Cholesterol crystals, the main component of human gallstones, are of interest to medical research as their structural properties can shed light on the pathologies of gallbladder. With our application we show that *ab initio* calculations can be employed to aid NMR crystallography.

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