

Abstract Submitted
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Interpreting magnetic resonance experiments from first principles CHRIS PICKARD, University of Cambridge, JONATHAN YATES, Lawrence Berkeley National Laboratory, SIÂN JOYCE, University of Cambridge, FRANCESCO MAURI, Université Pierre et Marie Curie — A method for predicting the results of magnetic resonance (NMR/EPR) experiments will be presented. It is based on the plane wave pseudopotential method, within density functional theory. Using a modified (gauge including) version of the projector augmented wave method, all-electron accuracy can be achieved. I will describe how the method is being adopted by the experimental community to assist in the extraction of the maximum amount of information from their magnetic resonance experiments. The range of applicability of the method will be emphasized, by reference to successful collaborative applications: porphyrin molecules, boron carbides, complex zeolite silicates, zircon, sodium and calcium silicate glasses and hydrogen bonded molecular crystals.

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