

Abstract Submitted
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Alternative approach to ab-initio NMR spectra for periodic systems TIMO THONHAUSER, Rutgers University/Massachusetts Institute of Technology, ARASH MOSTOFI, NICOLA MARZARI, Massachusetts Institute of Technology, DAVID VANDERBILT, Rutgers University, RAFFAELE RESTA, University of Trieste — We propose a novel finite-differences approach for computing the NMR response in periodic solids that is based on the theory of orbital magnetization¹ recently introduced by some of us. Instead of obtaining the shielding tensor from the response to an external magnetic field, we derive it directly from the orbital magnetization appearing in response to a microscopic magnetic dipole. This procedure has an established parallel in the case of electric fields, where Born effective charges are often obtained from the polarization induced by a sublattice displacement instead of the force induced by an electric field. Among the advantages of the present approach are its simplicity and its applicability to situations in which linear-response theory would be cumbersome.

¹T. Thonhauser, D. Ceresoli, D. Vanderbilt, and R. Resta, Phys. Rev. Lett. **95**, 137205 (2005).

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