MAR08-2007-000320

A converse approach to the calculation of NMR shielding tensors

TIMO THONHAUSER, Massachusetts Institute of Technology

We propose an alternative approach for computing the NMR response in periodic solids that is based on a recently developed theory of orbital magnetization [1]. 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 [2]. Our new approach is very general, and it can be applied to either isolated or periodic systems. The converse 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. Our novel approach is simple and straightforward to implement since all complexities concerning the choice of the gauge origin are avoided and the need for a linear-response implementation is circumvented. We have demonstrated its correctness and viability by calculating chemical shieldings in simple molecular systems, finding excellent agreement with previous theoretical and experimental results. Applications to more complex systems are currently in progress.

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

(2) T. Thonhauser, Arash A. Mostofi, Nicola Marzari, R. Resta, David Vanderbilt, submitted to Phys. Rev. Lett. (2007), arXiv:0709.4429v1.