

Ab Initio Calculation of Indirect Spin-Spin Coupling Constants

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Indirect spin-spin, or “J-coupling” constants have been of considerable use for extracting detailed structural information from high-resolution NMR spectra. We present here a method for calculating all four contributions from the nonrelativistic Ramsey theory; the dia- and para-magnetic contributions along with the Fermi-contact and spin-dipolar contributions. Our method is based on the so-called “converse” method for NMR [1] and computes the necessary energy second derivatives directly using a numerical finite-differences scheme, therefore eliminating the need for a complex linear response framework. We have implemented our method as part of a plane-wave density functional theory code using pseudopotentials.

[1] T. Thonhauser *et al.*, Phys. Rev. B **81**, 184424 (2010).