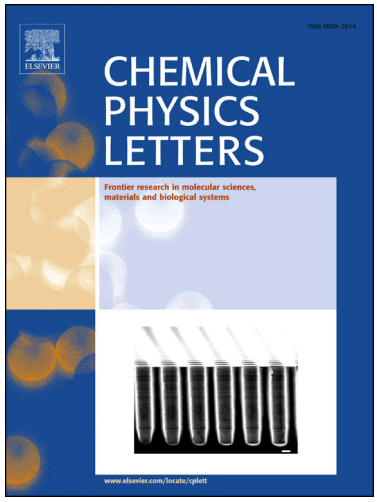

Research paper

An Extrapolation Scheme for Solid-State NMR Chemical Shift Calculations

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An Extrapolation Scheme for Solid-State NMR Chemical Shift Calculations

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Abstract

Conventional quantum chemical and solid-state physical approaches include several problems to accurately calculate solid-state nuclear magnetic resonance (NMR) properties. We propose a reliable computational scheme for solid-state NMR chemical shifts using an extrapolation scheme that retains the advantages of these approaches but reduces their disadvantages. Our scheme can satisfactorily yield solid-state NMR magnetic shielding constants. The estimated values have only a small dependence on the low-level density functional theory calculation with the extrapolation scheme. Thus, our approach is efficient because the rough calculation can be performed in the extrapolation scheme.

Keywords: Solid-state NMR; Chemical shifts; Extrapolation scheme.