

RELATIVISTIC XE CHEMICAL SHIFT IN CARBON NANOTUBES

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Xenon guests are used intensively in NMR spectroscopy as spy atoms in various materials due to its inertness and highly sensitive NMR chemical shift. It provides detailed experimental information of material properties of, e.g., porous solids [1].

Theoretical description of Xe chemical shift inside fullerenes is shown to necessitate inclusion of both relativistic and dynamic effects [2]. The recently developed Breit-Pauli perturbation theory (BPPT) [3] of leading-order relativistic effects on nuclear shielding enables the inclusion of electron correlation effects on the Xe shift. This is so far the only method by which ab initio electron-correlated relativistic shieldings are available. By using BPPT, the correlation effects, especially in the nonrelativistic part of the shielding tensor, have been found to constitute a challenge for the present DFT methods in xenon compounds such as xenon fluorides [4] and the novel HXeCCH molecule [5]. Quantitative theoretical description of the experimentally probably best-characterized intermolecular interaction effect in NMR, the temperature dependence of the second virial coefficient of ¹²⁹Xe shielding, was reached by including both relativistic and high-level electron correlation effects in the binary Xe chemical shift function [6].

In the present work, previous experience is exploited in the theoretical description of Xe NMR shift in single-wall carbon nanotubes (SWCNT). The dependence of relativistic Xe shift on the adsorption site both inside and outside the nanotubes is settled. Also the sensitivity of the Xe shift to the SWCNT type is explored.

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