Contribution ID: **47** Type: **Poster (In person)**

NMR shielding calculations –from accurate nuclear magnetic moments to interpretation of NMR spectra

Wednesday 29 November 2023 18:00 (1 minute)

Beta-detected nuclear magnetic resonance (β-NMR) is a sensitive technique, which has gained widespread recognition in the fields of nuclear physics [1] and materials science [2]. The recent utilization of ionic liquid targets has unlocked fresh opportunities for incorporating β-NMR spectroscopy into the domain of chemistry [3]. Precise determinations of the nuclear magnetic moments of β-NMR probes enable the direct evaluation of NMR shielding in β-NMR experiments [4]. Nevertheless, the successful execution of these experiments relies also on robust ab initio modeling support. In this study, we present a computational methodology for ascertaining the NMR shielding of β-NMR probe nuclei in ionic liquids and water environment. Our approach entails the use of force-field molecular dynamics to simulate the solvation shell structure, subsequently employing approximate models for NMR shielding. These models are based on non-relativistic coupled cluster and four-component Dirac-Kohn-Sham methods. Through benchmark calculations,we have observed that the proposed NMR shielding models can accurately predict the NMR shielding of alkali metal ions (Li+, Na+, K+) within ionic liquids and water with an accuracy of just a few parts per million (ppm). The calculated NMR shieldings can be used in re-derivation of nuclear magnetic moments or could serve as a computational support for interpretation of measured β-NMR spectra.

[1] G. Neyens et al.,Physical Review Letters 94, 022501 (2005)
[2] D. Cortie et al.,Physical Review Letters 116, 106103 (2016)
[3] R. McFadden et al.,Angewandte Chemie International Edition 61, 35 (2022)
[4] R. Harding et al.,Physical Review X10, 041061 (2020)

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Session Classification: Poster Session