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Using computational simulations to support structural characterization of metals, alloys, and intermetallic compounds with solid-state NMR

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The use of solid-state nuclear magnetic resonance (ssNMR) spectroscopy in materials science has boomed in recent years. What makes it a new valuable tool for the development of the next generation of materials, providing new insights into atomic arrangement and electronic structure of solid samples. Naturally, there is no denying that this is mainly due to advances in ssNMR techniques and the high-resolution spectra that can be obtained nowadays. Nevertheless, one cannot rule out the important role of density functional theory (DFT) based computational simulations in that context. With a highlight to the gauge-including projector augmented-wave (GIPAW) method.

It is nothing new that the aid of DFT-GIPAW calculations may be crucial for unambiguous ssNMR peak assignments in a number of cases. Whether it is a matter of structural intricacy like static disorder, mixture of phases, or chemical exchange processes; or due to a combination of distinct magnetic screening mechanisms (MSMs) resulting from different aspects of the electron charge and spin densities around target nuclei. That combination of MSMs is precisely one of the biggest challenges in the interpretation of the spectra of materials in which, in the presence of the applied external magnetic field, electrons define the local environment of target nuclei behaving not only as moving charges, but also as particles with spin ½.

With a focus on the 27Al nuclide in weakly magnetic intermetallic compounds and in a bulk glass alloy, the aim of the current research is to show that DFT-GIPAW calculations of orbital and Fermi-contact shifts can not only promote a less unbiased interpretation of the respective ssNMR spectra, but also demonstrate the possibility of expanding out the applicability of that type of spectroscopy to a new class of materials.

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