NMR Shielding Tensors and Shifts in the Local Exact Two-Component Theory

Yannick J. Franzke[a] and Florian Weigend[b]

[a] *Institute of Physical Chemistry, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany*
[a] *Institute of Nanotechnology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany*

An efficient implementation of scalar-relativistic NMR shielding tensors based on the one-electron spin-free exact two-component theory (X2C) is presented [1]. It utilizes the finite nucleus model and takes advantage of the diagonal local approximation to the unitary decoupling matrix (DLU). This allows for routine calculations of large molecules with heavy atoms. Efficiency is demonstrated for heavy-element clusters and organometallic complexes with more than 120 atoms. The accuracy of the DLU scheme is evaluated based on NMR shielding constants and chemical shifts of C, O, Si, Ge, Sn, Xe, W and Pb. Further, extensions for the all-electron relativistic Karlsruhe basis sets [2] are presented. These extensions require at most four additional primitive basis functions. A large set of more than 250 closed-shell molecules was used to assess the quality of the developed extensions throughout the periodic table of elements.

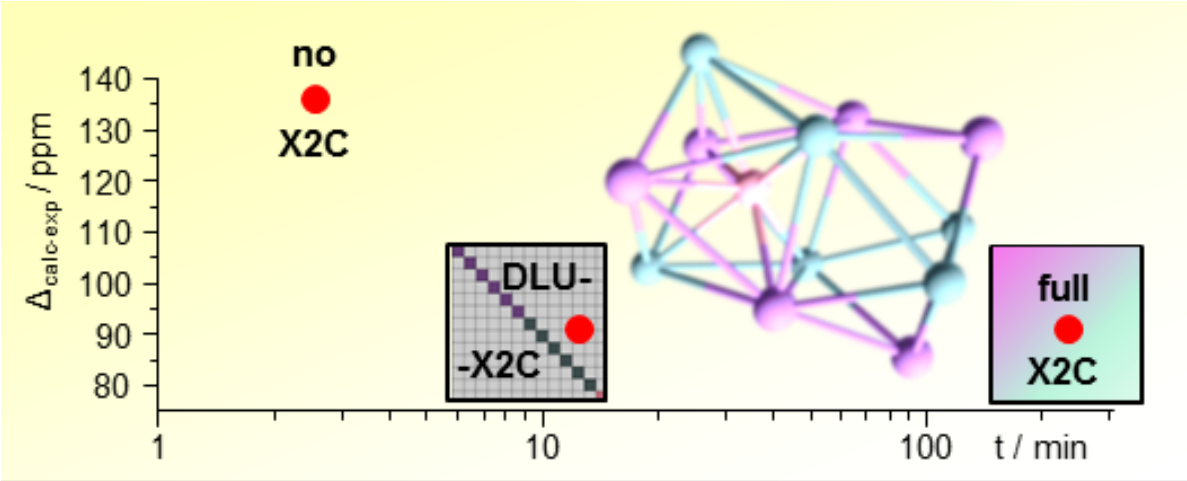

Figure 1: Accuracy and efficiency of DLU-X2C versus full X2C and non-relativistic treatment for Sn-119 NMR shifts in $[Co@Sn_6Sb_6]^{3-}$.

References

1 Y. J. Franzke and F. Weigend, *J. Chem. Theory Comput.* **15** (2019), 1028.
2 P. Pollak and F. Weigend, *J. Chem. Theory Comput.* **13** (2017), 3696.