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Theory complements β-NMR studies: correlation time of 23Na+ in liquids

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The molecular environment around different ions in liquids and solids can be determined experimentally using the technique of β-NMR, based for example on the relaxation time T1. However, to interpret T1 correctly in liquids, one needs to take into account the underlying dynamics, which can be done by combining β-NMR results with calculations of the molecular correlation times. Several theoretical methods can be used, such as molecular dynamic (MD), density functional theory (DFT), or a combination of quantum mechanics with molecular mechanics (QM/MM).
To complement β-NMR studies on short-lived 26Na in different ionic liquid hosts, in the present work MD simulations have been applied to study the dynamics of water molecules around the Na+ ion (using the Amber software), before the application in ionic liquids. The obtained correlation time value is in good agreement with other computational results. This method can be now applied to other environments, like ionic liquids.
The poster will present the theoretical approach, the obtained results compared to literature values, and will present them in the context of β-NMR studies performed at ISOLDE.

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