Density functional theory studies on 1-butyl-3-methylimidazolium chloride

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Ionic liquids are a class of organic compounds which exhibit some peculiar properties including low vapour pressure, no volatility, thermal and chemical stability, electrical conductivity, and catalytic properties. They are also good solvents for polar and non-polar molecules. Ionic liquids are commonly used in laboratory as solvents in organic synthesis, extraction and chromatography. The electric conductivity and the diffusion ability of the ions can be tailored for application in fuel cells and batteries. There are many possible combinations of cations and anions, which makes it possible to fine-tune the chemical and physical properties to the desired application. Due to the rich set of possibilities it is beneficial to do computational studies to help the choice of a suitable molecule.

The properties of ionic liquids have been thoroughly studied both experimentally and computationally. One intriguing experimental technique is the analysing the internal structure of the bulk using the ^{129}Xe nuclear magnetic resonance (NMR) spectrum. The xenon atom is highly polarizable yet inert probe, which gives rise to large chemical shifts in the NMR spectrum. It was found that the size of the anion in the ionic liquid affects significantly the free volume, which correlates with the solvation ability of the molecule.

The theoretical study involves obtaining the optimized geometries of clusters of the ionic liquid with a xenon atom at DFT level, and calculating the nuclear shieldings to predict the ^{129}Xe NMR spectrum using ZORA. The first part of the study involves obtaining the geometry of the ionic liquid cluster at the PBEh-3c/def2-mSVP/D3-BJ level of theory. The density functional allows calculations on extended systems within a reasonable time frame. After the structure was obtained, a xenon atom is added to different locations and the structures optimized further. The nuclear shielding calculations require that relativistic effects be taken into account for the xenon atom.