CLINT
CRC 1452 Catalysis at Liquid Interfaces

Guest Colloquium of the CRC 1452
CLINT ~ Catalysis at Liquid Interfaces

Describing ionic liquid systems: Partial charges, charge transfer and polarisability

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in lecture hall H3,

Egerlandstr. 3

and

Zoom Online Meeting

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Describing ionic liquid systems: Partial charges, charge transfer and polarizability

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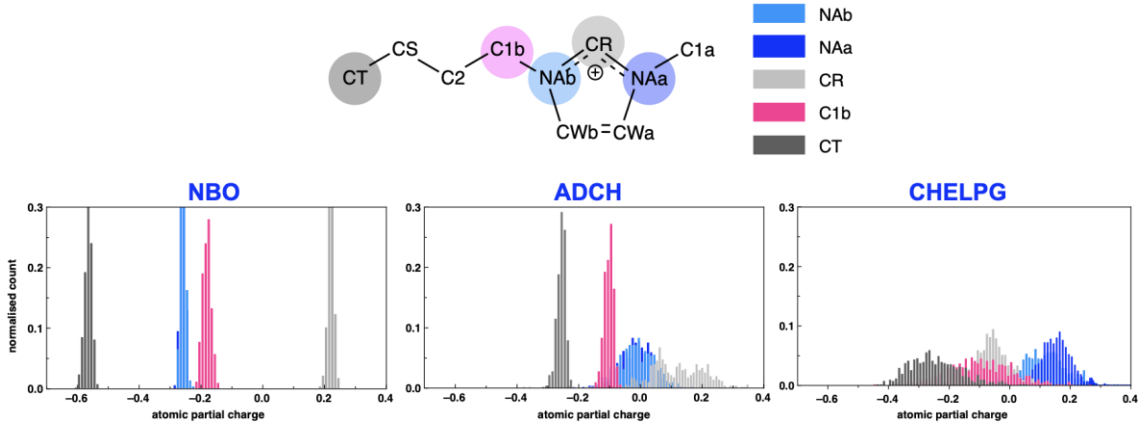
Ionic liquids (ILs) are of substantial interest for industrial applications, electrochemical devices (batteries) and as specialist engineering materials. In many cases the ionic nature of the IL is key, and how the ions respond to charge transfer as well as local or applied electric fields is critically important. Yet, how we conceive of the charge distribution within ILs, the impact of addition or removal of "charge" or the polarisation of charge in an electric field is often not well defined at the molecular level. Moreover, the predictive and explanatory power a molecular dynamics simulation is linked to the quality of the underlying force field, in which the charge distribution is vitally important.

In this talk I will focus on the iconic and widely employed $[C_4C_1im][NTf_2]$ (1-butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide) IL. The charge distribution within the ions, and impact of charge transfer will be considered. The variation in atomic partial charge for different sampled conformers for different methods of evaluation have been compared. I will explore the origins of why qualitatively different charges can be delivered for different methods. Within ILs charge transfer is known to occur, and a standard approach is to uniformly scale all charges, however individual atoms have a different hardness and this approach may not always be suitable. We have developed an interpolation method for determining atom-wise scaled partial charges and compared simulations based on the atom-wise scaled charges with others based on uniformly scaled and fully polarisable Drude particles. Overall, we find that there are still a number of challenges to be overcome when considering charge models for this proto-typical ionic liquid.



Partial charges determined from 500 sampled conformers of $[C_4C_1im]^+$ from a natural bond orbital (NBO), atomic dipole moment corrected Hirshfeld (ADCH) and charges from electrostatic potentials using a grid-based method (CHELP) analysis.