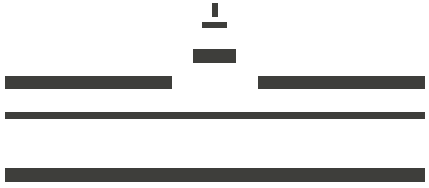

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FORCONX & POLARIZABLE MD-SIMULATIONS

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Motivation of the STSM

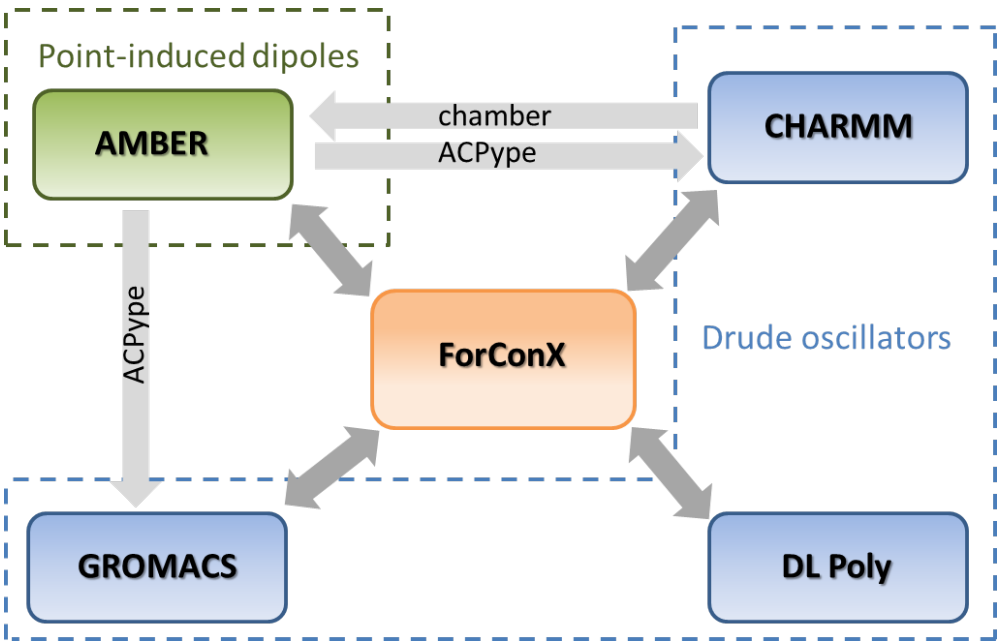
- Many different formats for force fields
- Each MD package has own input structure
- Conversion is error-prone and tedious

→ **Development of a conversion tool**

- Polarizable MD-simulations take care of electron cloud
- Two polarization methods are mainly used
- Drude oscillators and induced point dipoles

→ **Can both methods be mapped onto each other?**

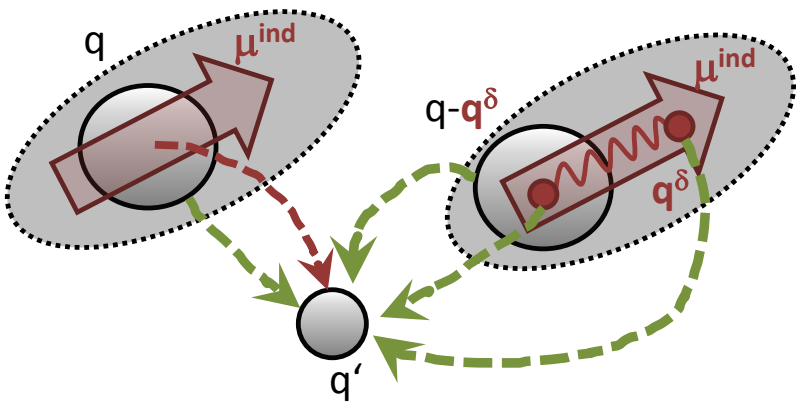
ForConX



- FORce field CONversion tool based on XML
- Easier access to MD-simulation
- XML structure as pivot
- XML for building up a database for ILs

The two polarization methods

(a) Point-induced dipoles (b) Drude oscillators



Drude oscillators (DRU)

- CHARMM
- Additional Drude particle
  - Charge, force constant
- Parameters: $\alpha_i = \frac{1}{4\pi\epsilon_0}\frac{(q_i^{\delta})^2}{k_i}$

Induced point dipoles (IPD)

- AMBER
- Implementation difficult
- Hydrogen polarization
- Parameters: polarizability α_i

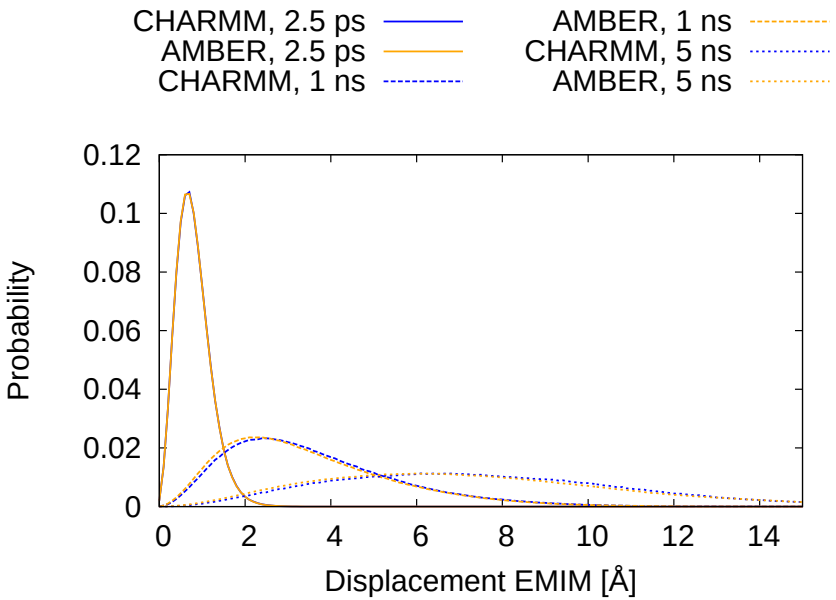
Is it possible to map both polarization methods onto each other?[1]

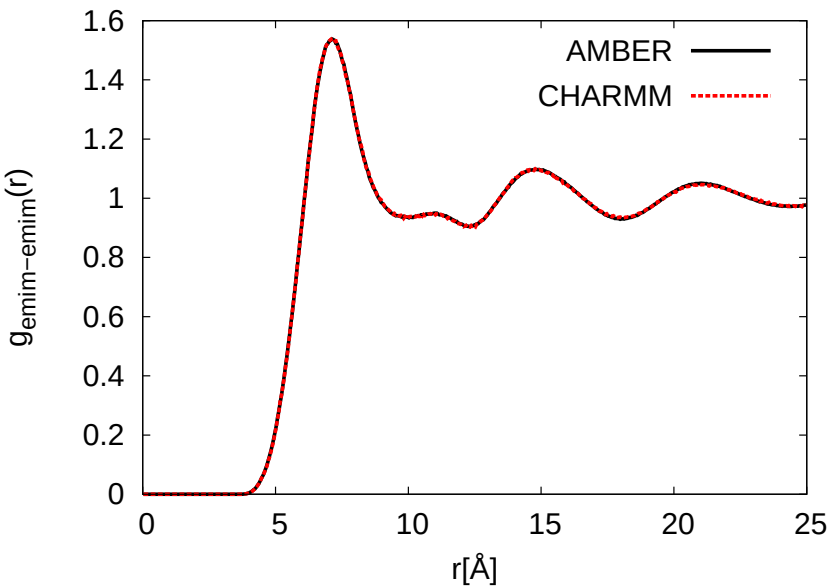
[1] Schmollngruber et al., PCCP, DOI: 10.1039/C4CP04512B, 2015.

Simulation details

- Cation: 1-ethyl-3-methylimidazolium
- Anion: Triflate
- Charmm (c37b1) and Amber (version 11)
- Fixed Drude charges ($q = 2e$)
- Four polarization models
  - Nonpol - non-polarizable MD-simulation
  - No H - hydrogen atoms are non-polarizable
  - Imp H - hydrogen polarizability shifted to next heavier atom
  - Exp H - full polarization (only IPD)

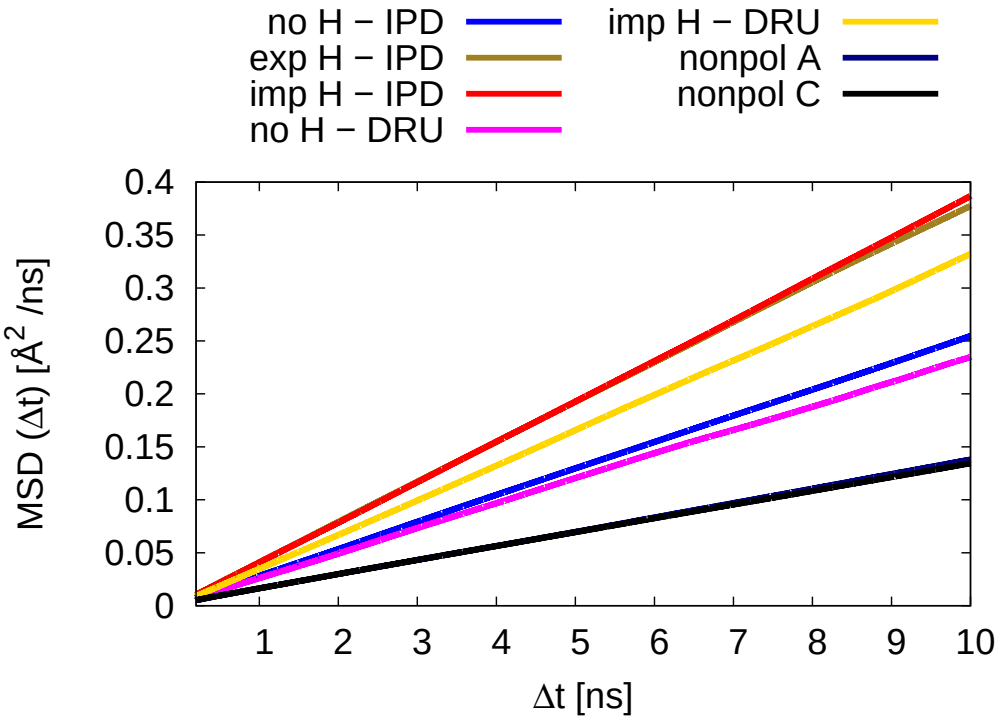
Excellent agreement for non-polarizable MD-simulations





$\Longrightarrow$ Excellent agreement for both structural and dynamical properties

Mean-square displacement



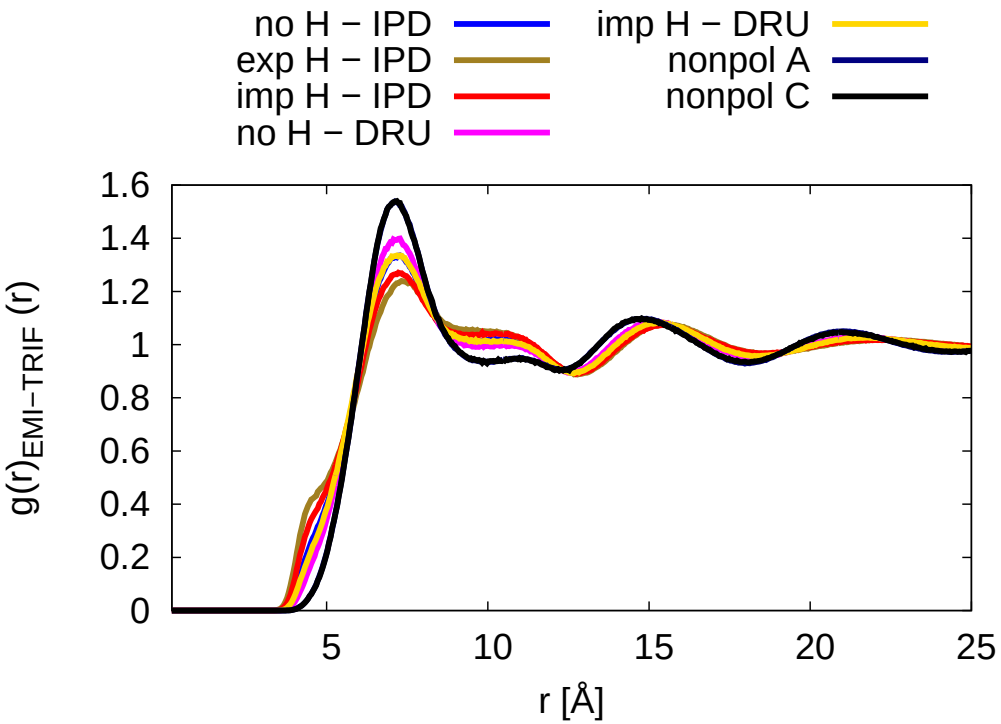
IPD Imp H and Exp H are similar to each other

DRU Imp H is slowed down, "no H" also slower than IPD

Imp H leads to high polarizabilities → Approximations in DRU model not longer valid

Imp H and Exp H show similar MSD → Hydrogen polarizability has to be present independent from location

Radial distribution function



IPD Small shoulder is more pronounced for higher polarizabilities

- Imp H (DRU) and no H (DRU) similar
- All polarization models similar for distances greater 10 Å

→ Hydrogen polarizability important for short range interaction

Summary

ForConX	XML structure should help to set up database
ForConX	Easier access to MD-simulation
Polarization	Non-polarizable simulations show good agreement
Polarization	Imp H and exp H show similar MSD but structures on short distances is different
Polarization	RDF is similar for all polarization model for large distances
Polarization	Approximations in the DRU model are not valid for high polarizabilities

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NATIONALE PLATTFORM ELEKTROMOBILITÄT

cost
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Thank you for your attention!!