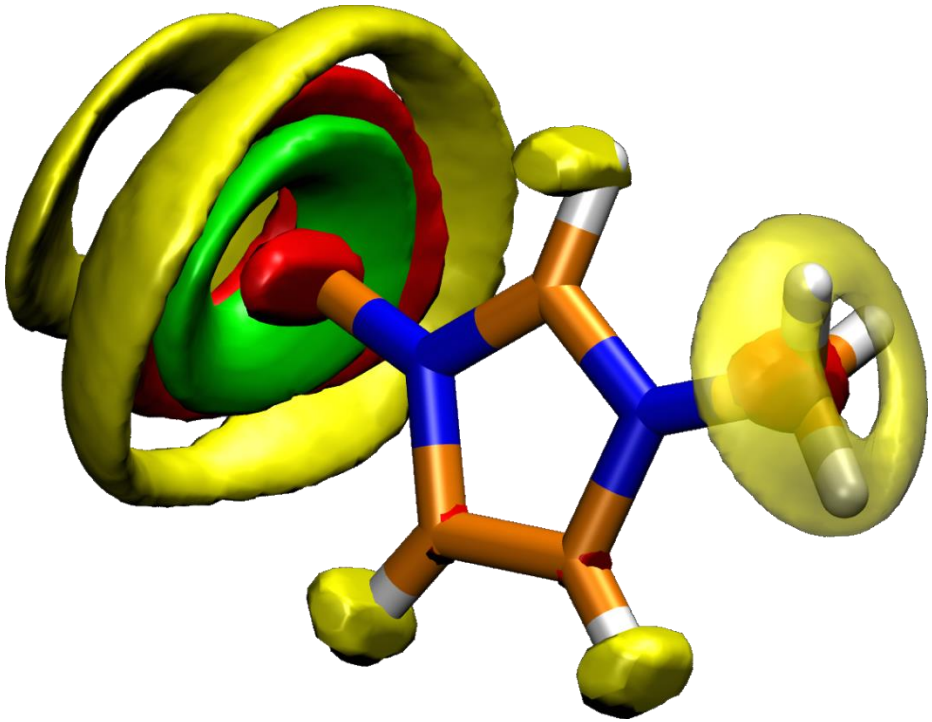
TRAVIS

A free Analyzer and Visualizer

for MC and MD Trajectories



http://www.travis-analyzer.de

Outline

1.) Introducing TRAVIS

2.) Some Exemplary Analyses

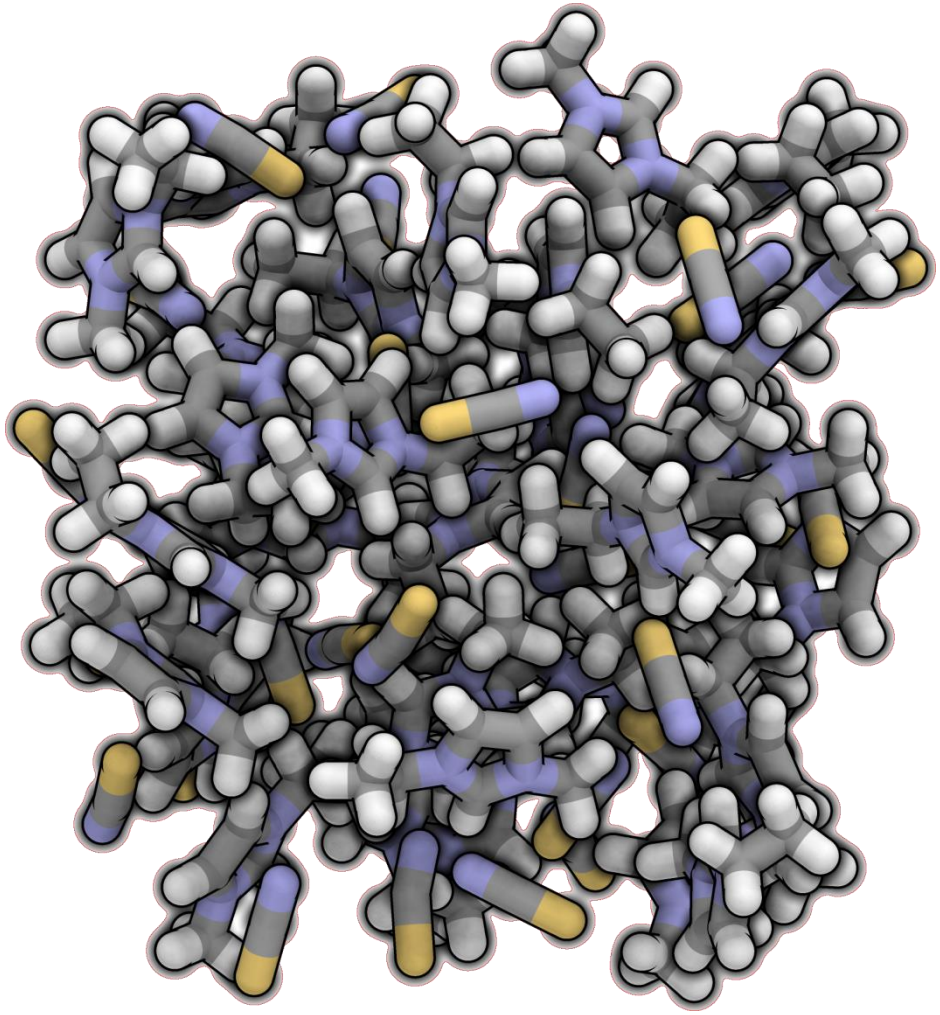
3.) Voronoi Charges

Analyzing Trajectories

- Direct result of all MD/MC simulations is a trajectory
- Contains positions and velocities of all atoms at each time

→ is a path through *6N*-dimensional space

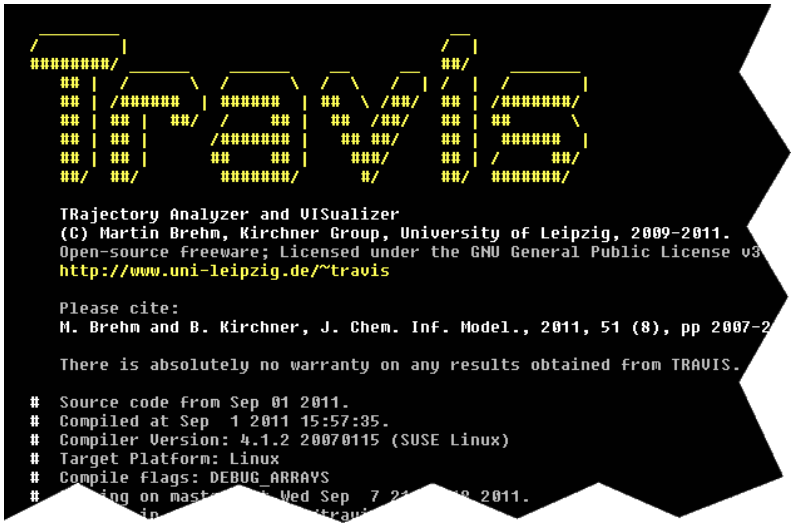
„Nice to look at, but cannot be evaluated directly.“



Mappings for the reduction of dimensionality are required.

Introducing TRAVIS

- Program package
  for doing these analyses
- Open-source free software;
  licensed under GNU GPL 3
- ≈ 290 000 lines of C++ code



- Platform independent (Windows / Linux / Mac)
- Published in 2011, cited more than 650 times since then:

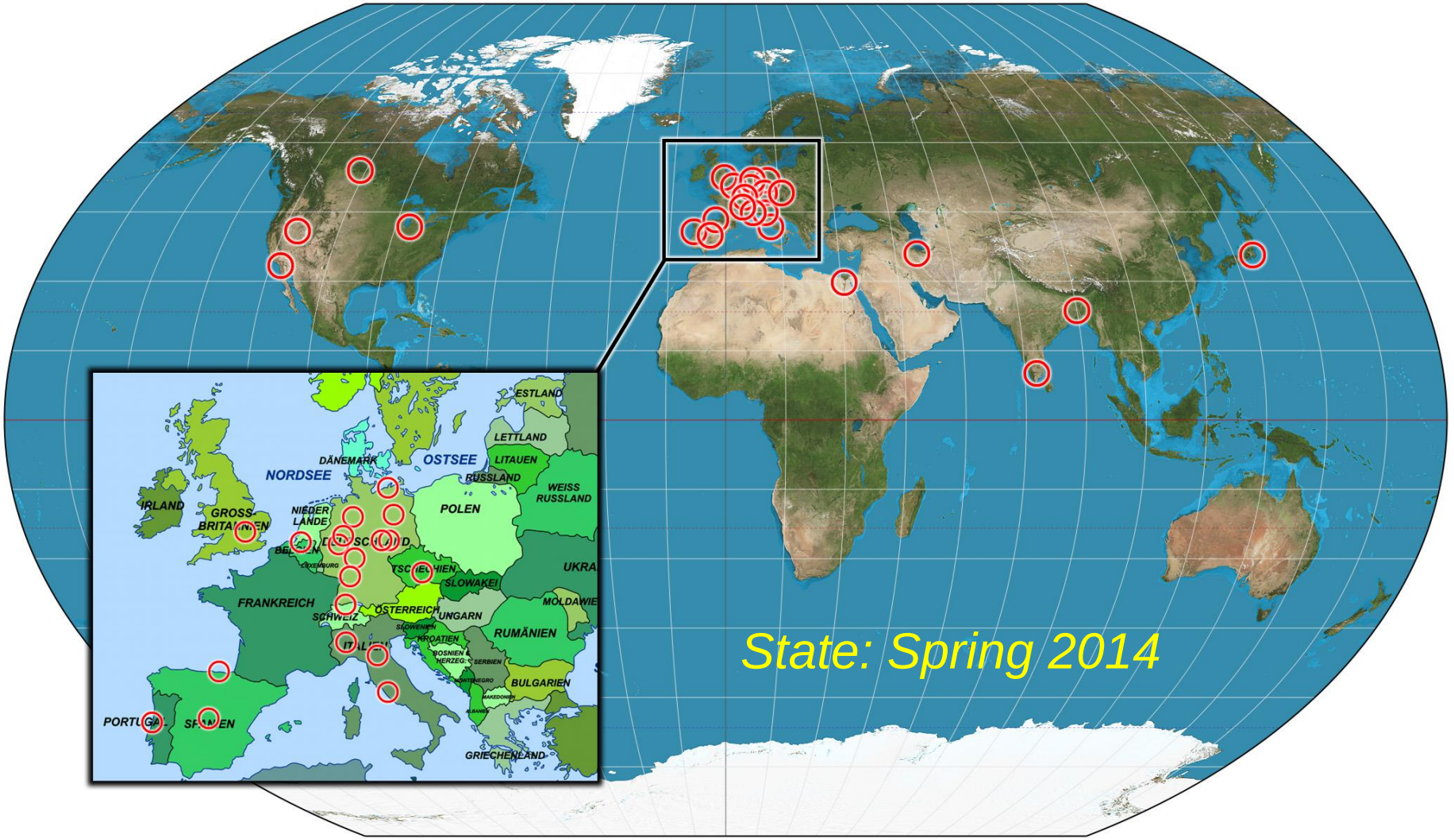
Martin Brehm and Barbara Kirchner: „TRAVIS - A Free Analyzer and Visualizer for Monte Carlo and Molecular Dynamics Trajectories“
J. Chem. Inf. Model. **2011**, *51 (8)*, 2007–2023 .

http://www.travis-analyzer.de

Introducing TRAVIS

Several dozen working groups around the world use TRAVIS

(I only know of the groups which had problems ☺)



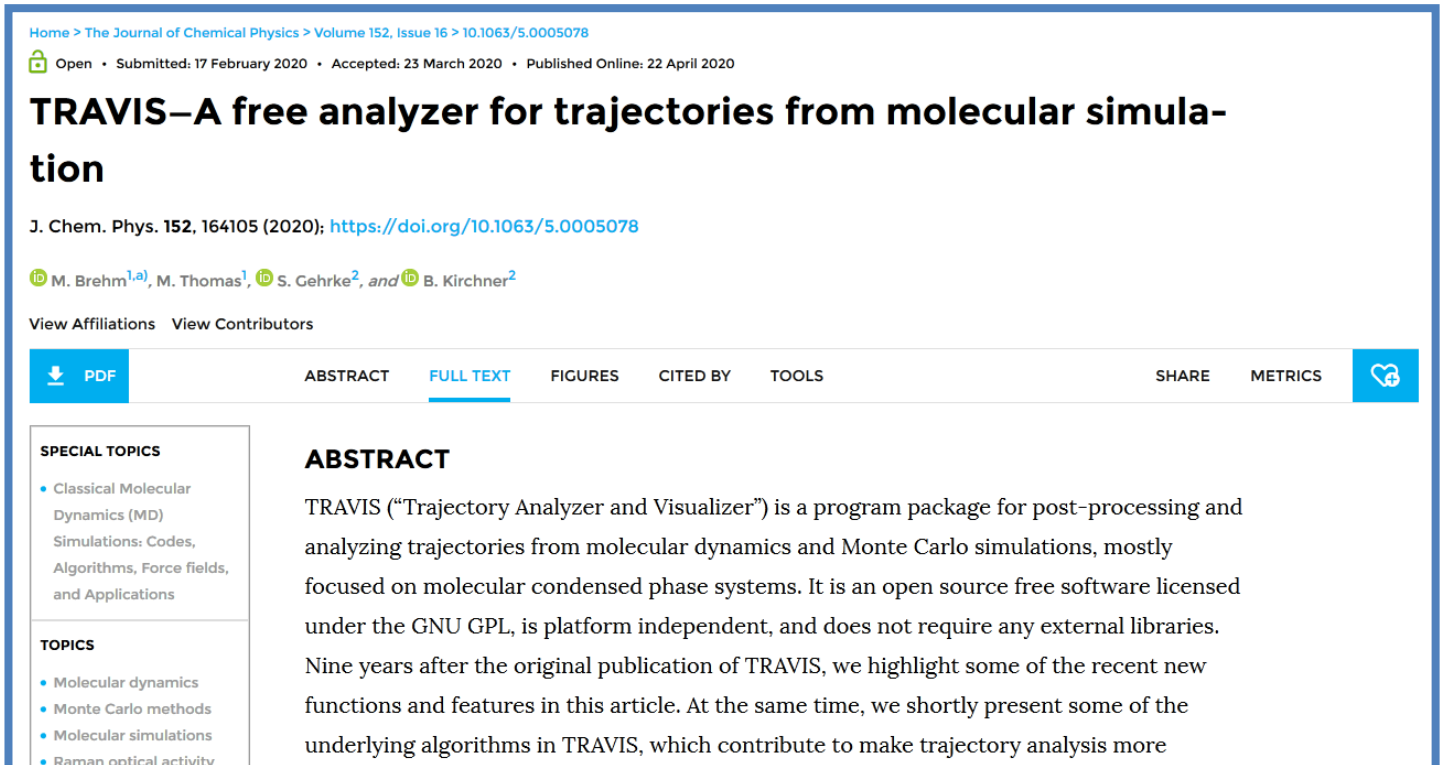
General Features

- Interactive text mode user interface (asks questions), but also scripting support
- Reads many popular trajectory file formats (xyz, pdb, mol2, AMBER, LAMMPS, DLPOLY)
- No limits on system size (works well with > 10^5 atoms)
- Support for periodic boundaries and changing cell vector (*e.g.*, from NpT simulations)
- Automatic molecule recognition (recognizes also molecules that are broken by wrapping)
- Atom labels based on purely topological algorithm

New Paper is out

In 2020, we published a new **open-access paper** on TRAVIS to show some of the newly added features:

M. Brehm, M. Thomas, S. Gehrke, B. Kirchner:
„TRAVIS – A Free Analyzer for Trajectories from Molecular Simulation“,
J. Chem. Phys. **2020**, *152 (16)*, 164105.



Home > The Journal of Chemical Physics > Volume 152, Issue 16 > 10.1063/5.0005078

Open • Submitted: 17 February 2020 • Accepted: 23 March 2020 • Published Online: 22 April 2020

TRAVIS–A free analyzer for trajectories from molecular simulation

J. Chem. Phys. 152, 164105 (2020); https://doi.org/10.1063/5.0005078

M. Brehm[1,a], M. Thomas[1], S. Gehrke[2], *and* B. Kirchner[2]

View Affiliations View Contributors

PDF ABSTRACT FULL TEXT FIGURES CITED BY TOOLS SHARE METRICS

SPECIAL TOPICS

- Classical Molecular Dynamics (MD) Simulations: Codes, Algorithms, Force fields, and Applications

TOPICS

- Molecular dynamics
- Monte Carlo methods
- Molecular simulations
- Raman optical activity

ABSTRACT

TRAVIS (“Trajectory Analyzer and Visualizer”) is a program package for post-processing and analyzing trajectories from molecular dynamics and Monte Carlo simulations, mostly focused on molecular condensed phase systems. It is an open source free software licensed under the GNU GPL, is platform independent, and does not require any external libraries. Nine years after the original publication of TRAVIS, we highlight some of the recent new functions and features in this article. At the same time, we shortly present some of the underlying algorithms in TRAVIS, which contribute to make trajectory analysis more

TRAVIS Citations by Feature

Go to **`https://brehm-research.de/travis`**

— Work Citing TRAVIS —

This is a list of publications which cite the **original TRAVIS article** from 2011.
Currently, there are **665** such publications, written by **1535** different authors.
634 out of these ***(95.34 %)*** actually used TRAVIS for results in the manuscript.

Go to Author List, go to Journal List.

Filter by TRAVIS Analyses...

665 citations in total. **Show continuous list view.**

	2011 *(3)*	2012 *(10)*	2013 *(10)*	2014 *(22)*	2015 *(37)*	2016 *(50)*	2017 *(61)*	2018 *(78)*	2019 *(101)*	2020 *(124)*	2021 *(126)*	2022 *(43)*	

— 2022 —

665 J. R. Avilés-Moreno, F. Gámez, G. Berden, J. Oomens, B. Martínez-Haya:
"Inclusion Complexes of the Macrocycle Nonactin with Benchmark Protonated Amines: Aniline and Serine"
Phys. Chem. Chem. Phys. **2022**, *accepted*. (DOI 10.1039/D2CP00264G) ⭳ Bib
Uses TRAVIS for Spec.

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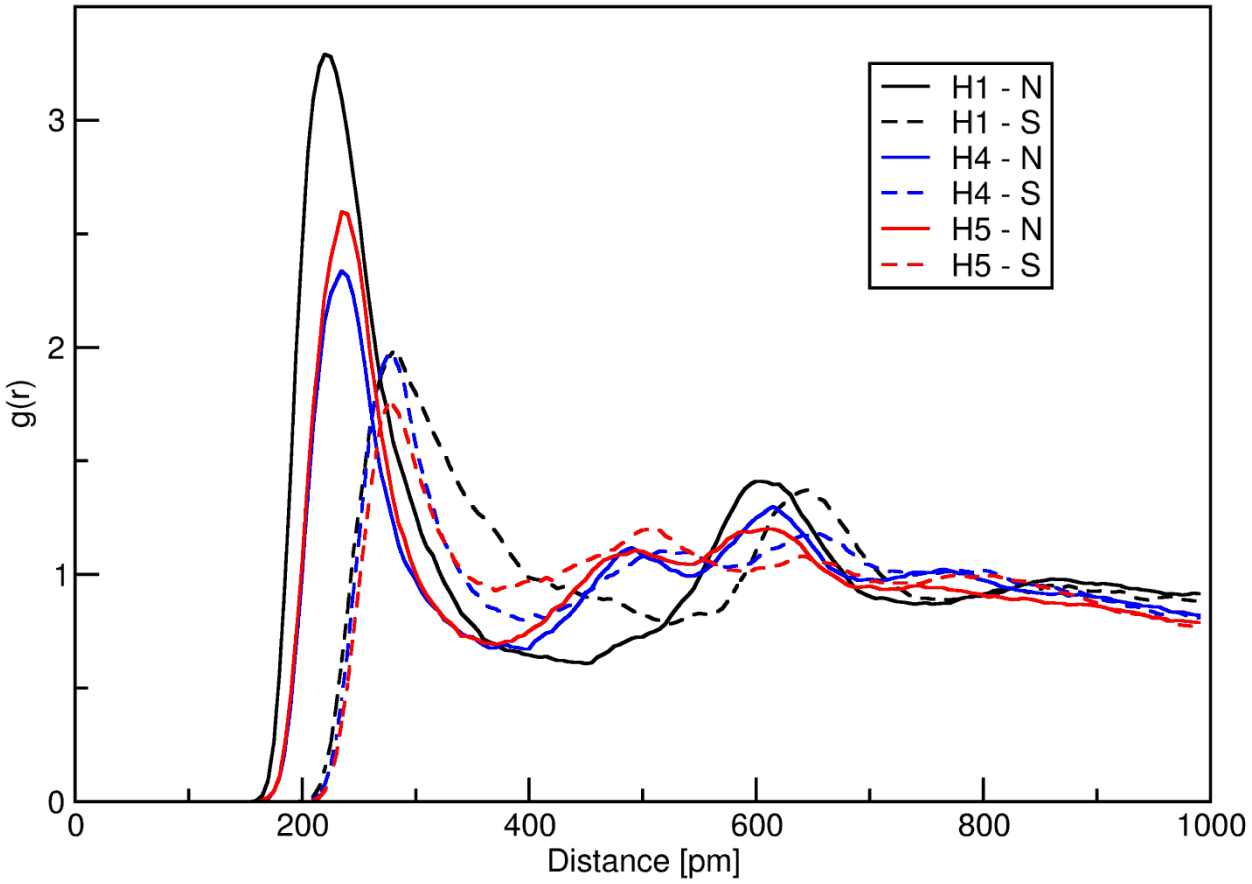
Show only articles where TRAVIS was used to compute...

- **... any result** ***(634)***
- **... RDFs (g(r), Radial Distribution Functions)** ***(263)***
- **... Number Integrals / Coordination Numbers** ***(72)***
- **... SDFs (Spatial Distribution Functions)** ***(313)***
- **... CDFs (Combined Distribution Functions)** ***(169)***
- **... 3D CDFs** ***(3)***
- **... Structure Factors / van Howe Correlations** ***(43)***
- **... Density Profiles** ***(19)***
- **... Aggregate Lifetimes (H Bonds, ...), Reactive Flux** ***(67)***
- **... MSDs (Mean Square Displacements), Diffusion Coefficients** ***(49)***
- **... Vector Reorientation Dynamics / Rotational Relaxation Times** ***(11)***
- **... Voronoi Statistics / Surface Coverage / Visualization** ***(18)***
- **... Voronoi-based Domain Analysis** ***(29)***
- **... Power Spectra / Vibrational Density of States** ***(58)***
- **... Vibrational Spectra (IR, Raman, VCD, ROA)** ***(66)***
- **... Bulk Phase Normal Modes** ***(7)***
- **... Order Parameters** ***(3)***
- **... Sankey Diagrams / Hydrogen Bond Topology** ***(5)***
- **... Connection Matrix** ***(3)***

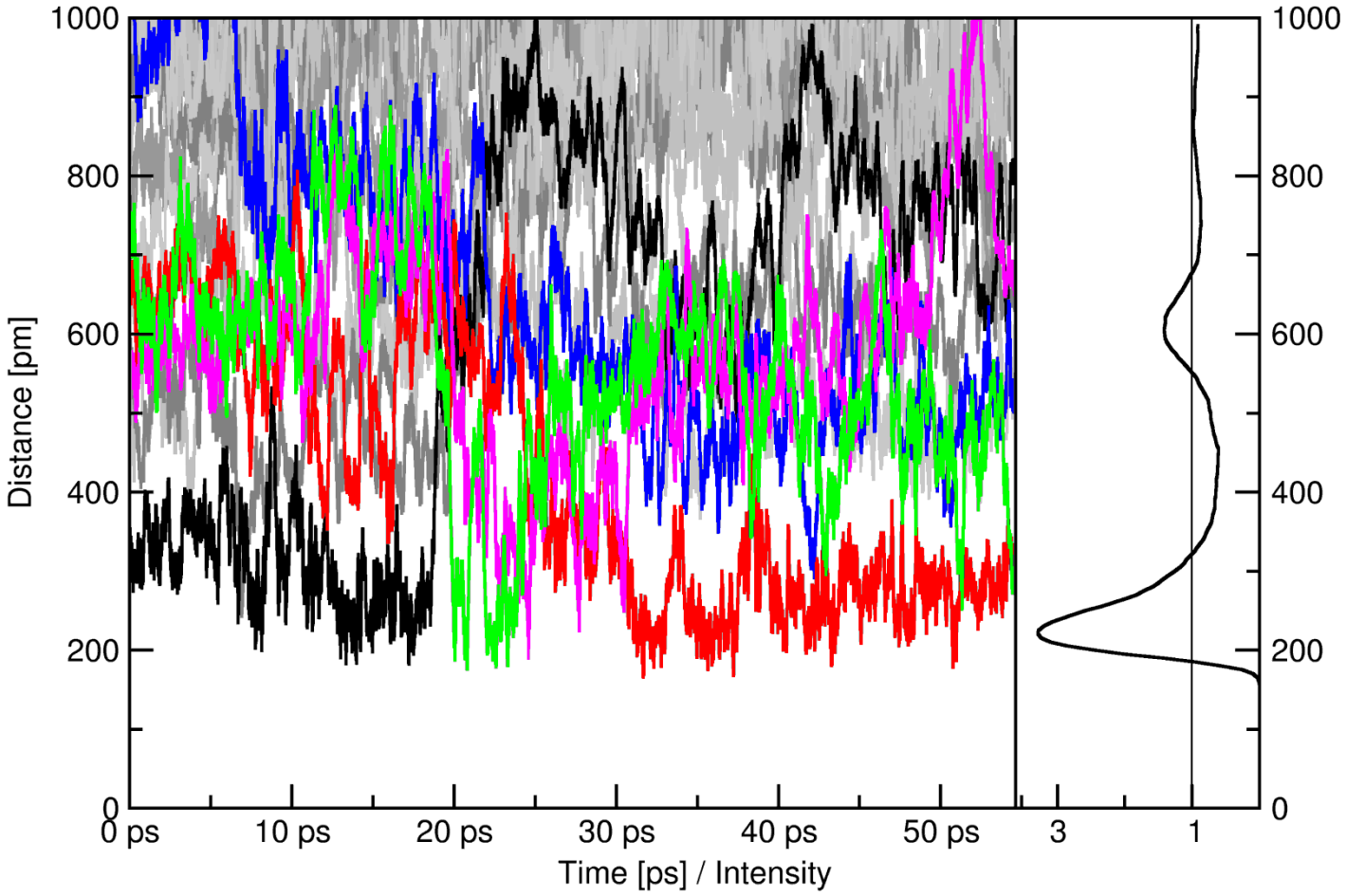
2.) Some Exemplary Analyses

Structural Analyses



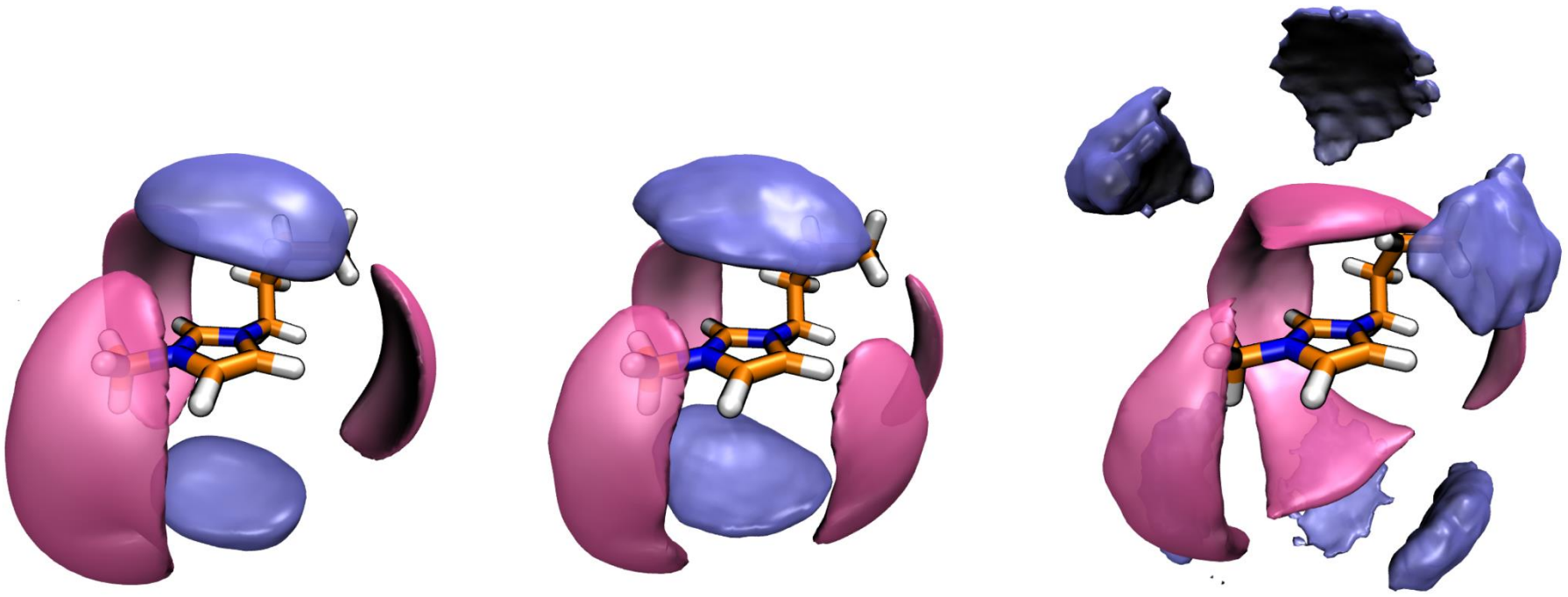
Radial Pair Distribution Functions

Structural Analyses



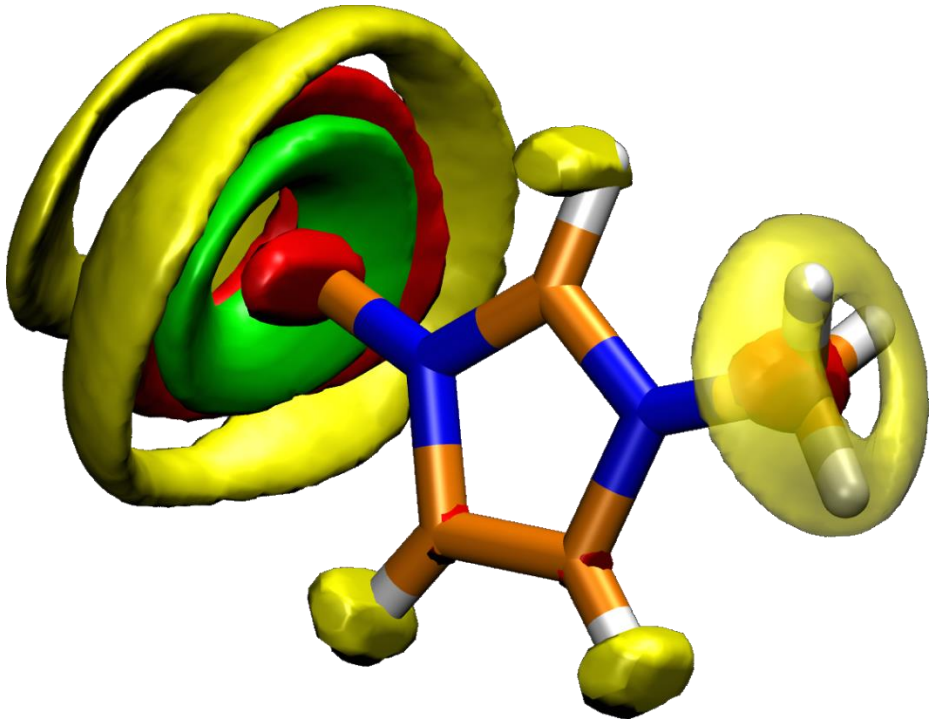
Temporal Distance Development and distribution

Structural Analyses



Spatial Distribution Functions

Structural Analyses



Spatial Distribution Functions

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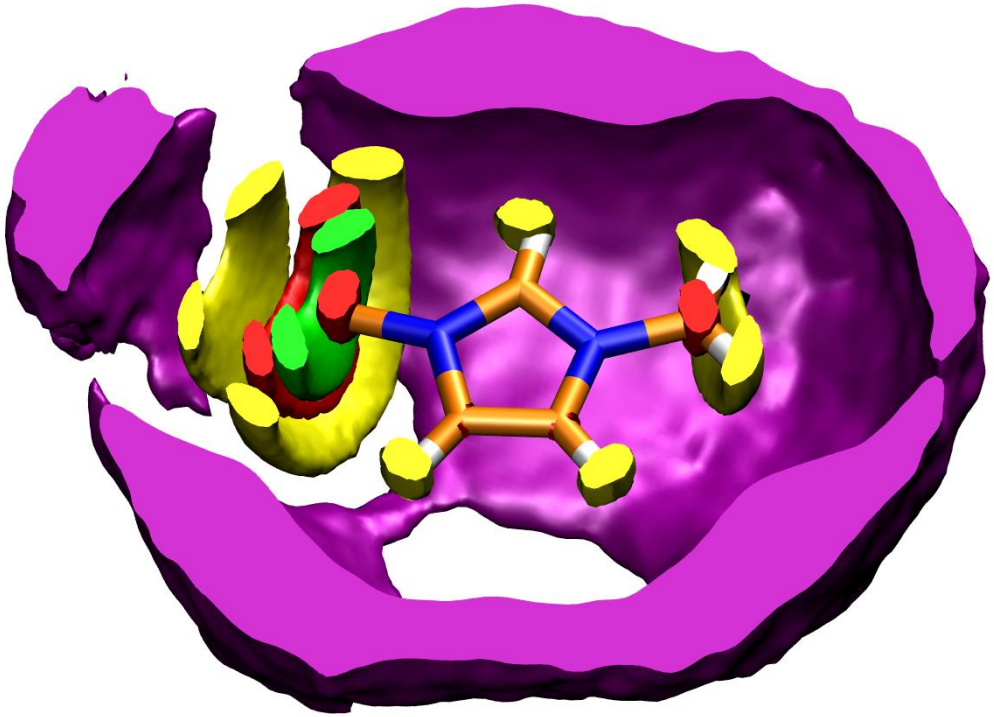

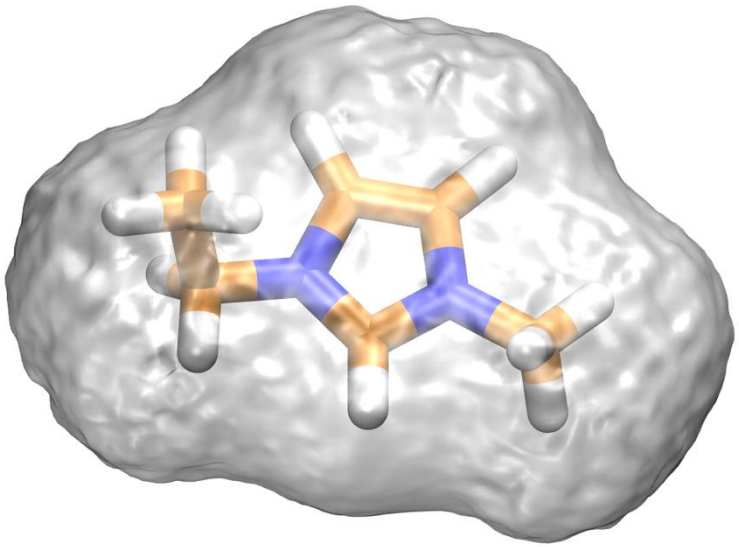

Spatial Distribution Functions

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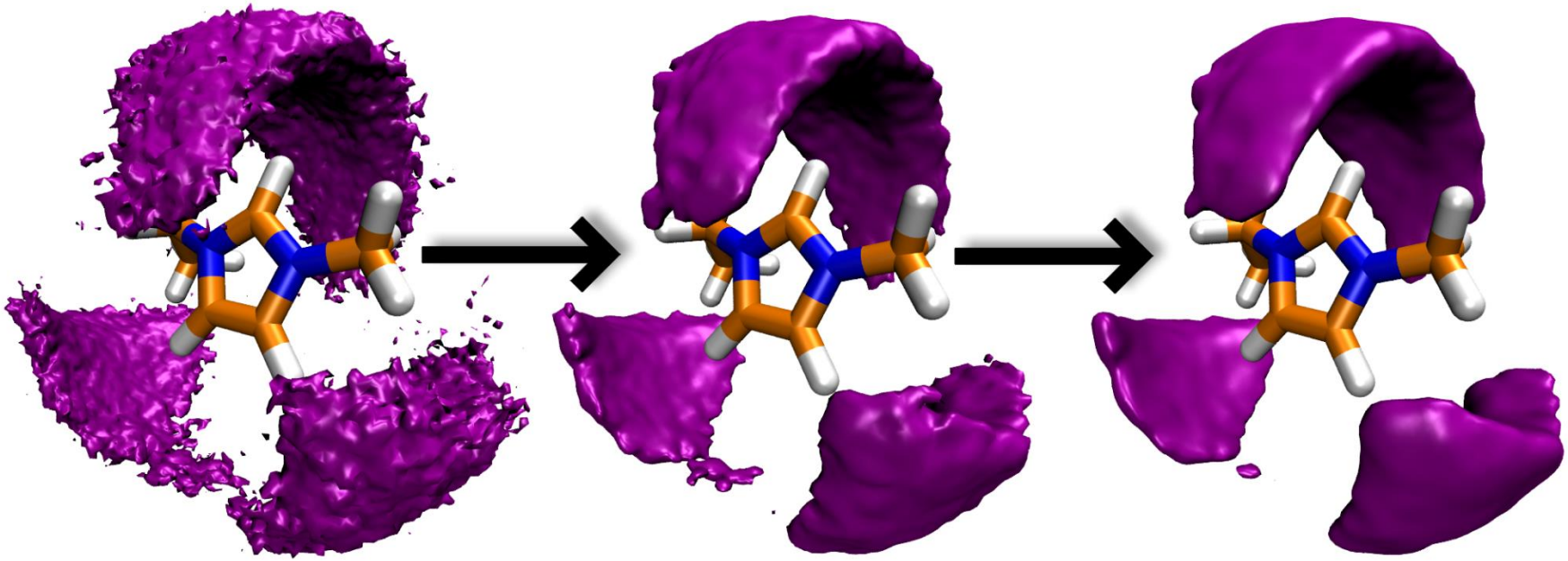
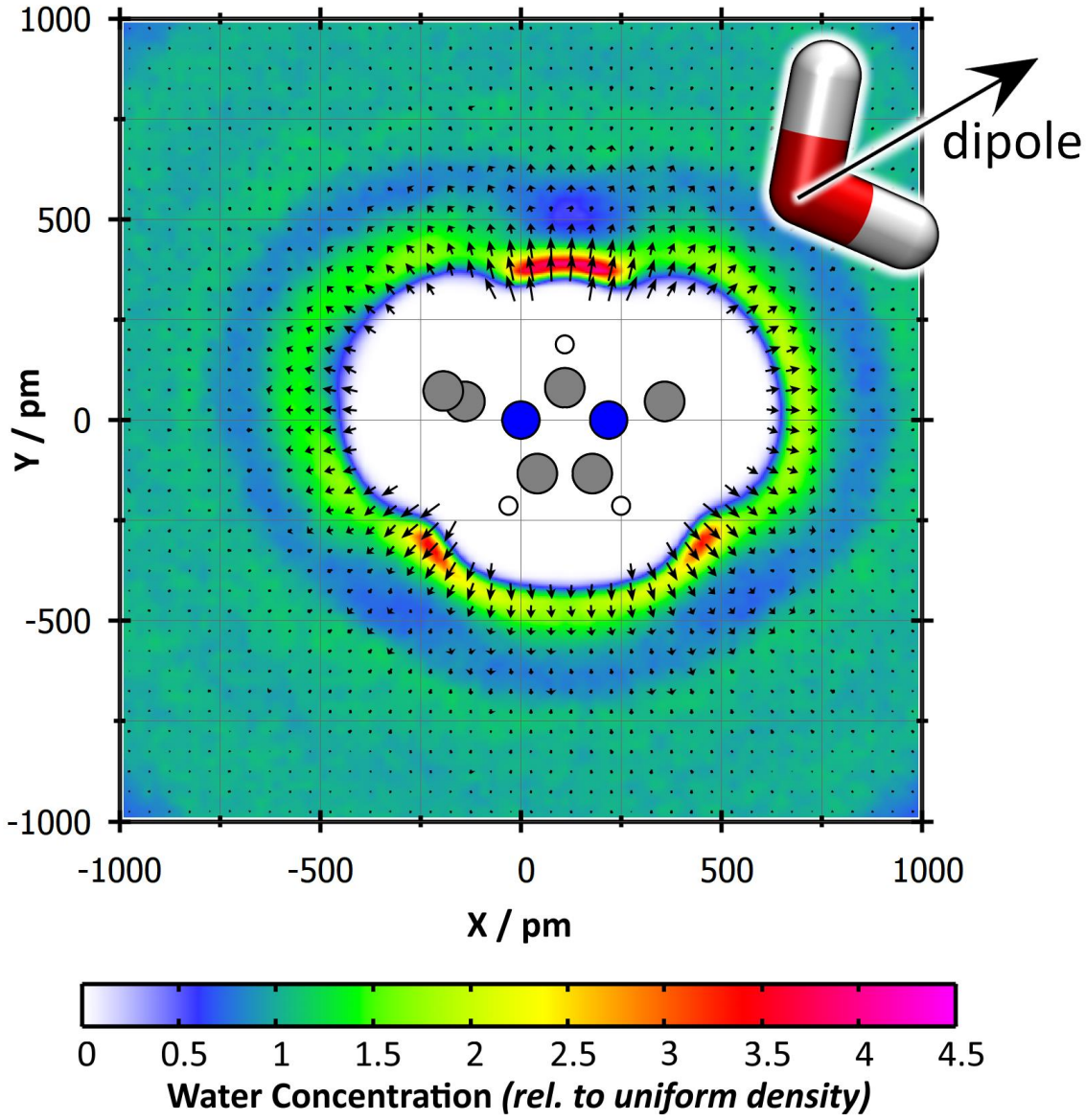


Smoothing of Spatial Distribution Functions

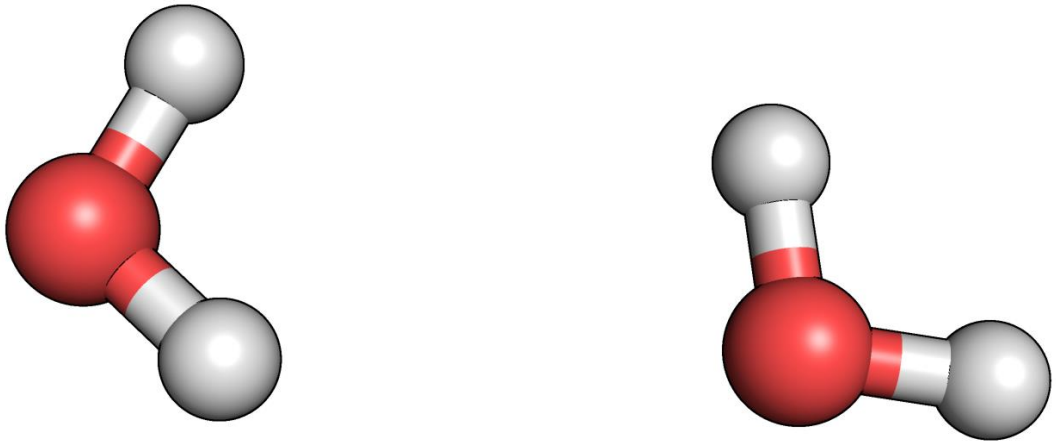
Plane Projection Analysis



Combined Distribution Functions

- One example for a new feature that did not appear in literature before

- Consider these 2 water molecules



- Define a distance and two angles

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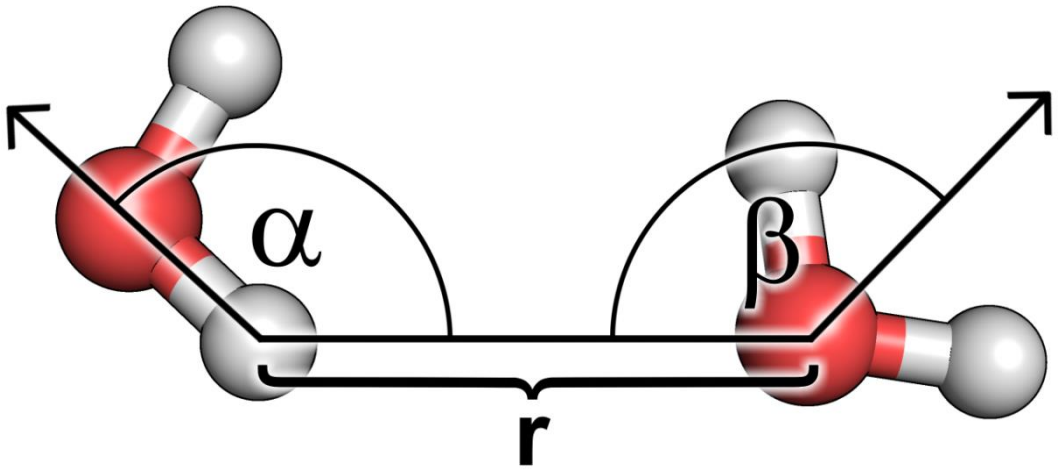
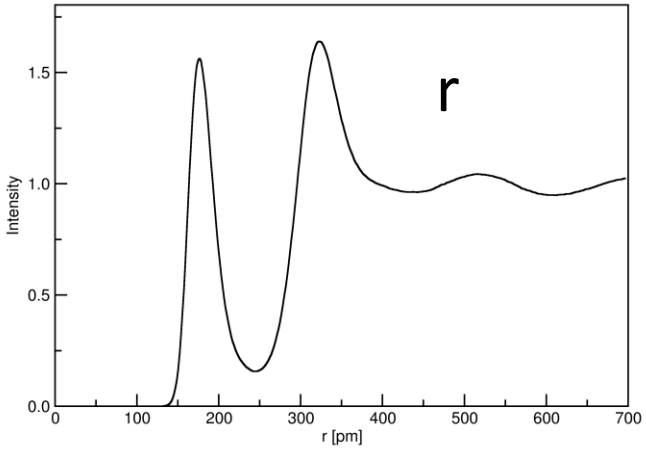
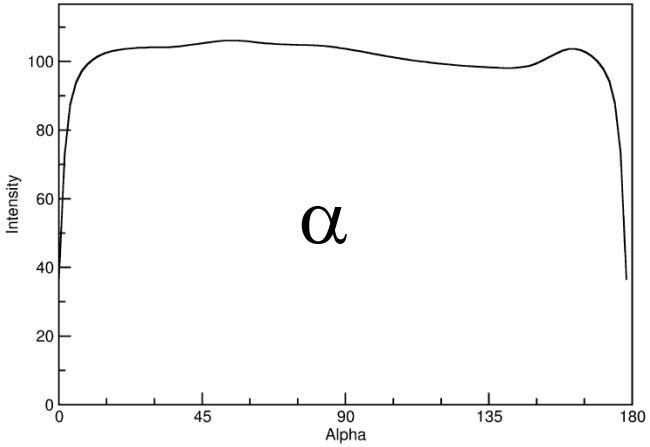


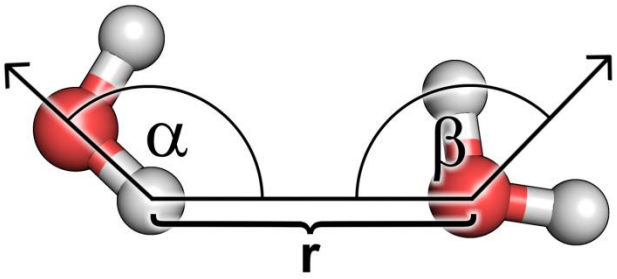
- Define a distance and two angles

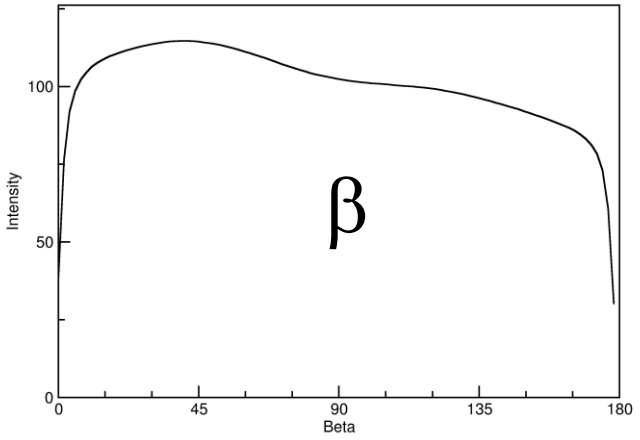
Combined Distribution Functions

- Plot distribution functions for these 3 quantities









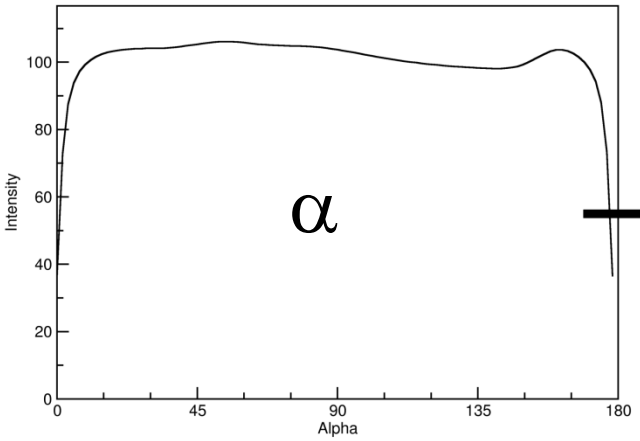
Combined Distribution Functions

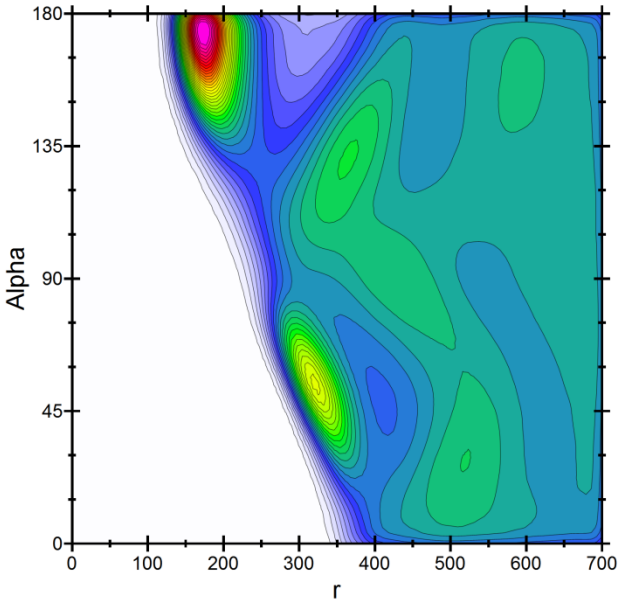
- So far nothing new

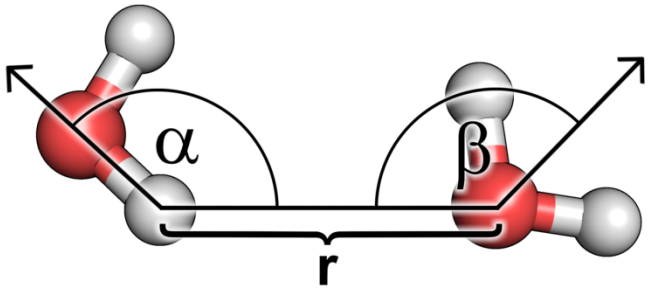
- Dependence of these quantities on each other is left out (but very important)

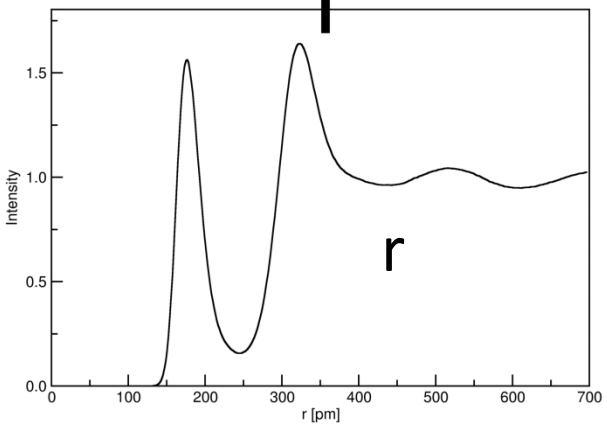
- Idea: Combine certain scalar quantities to yield Combined Distribution Functions (CDFs)

Combined Distribution Functions









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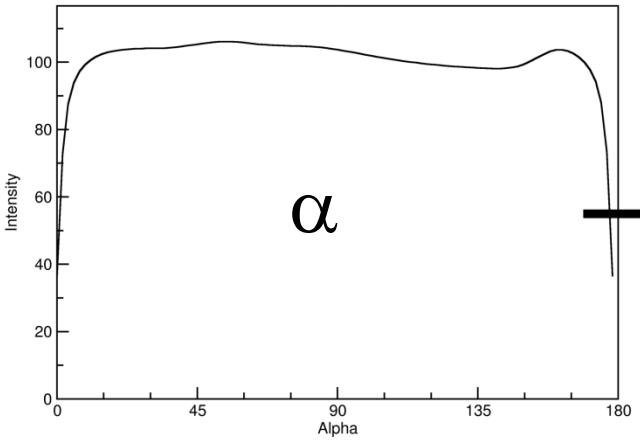

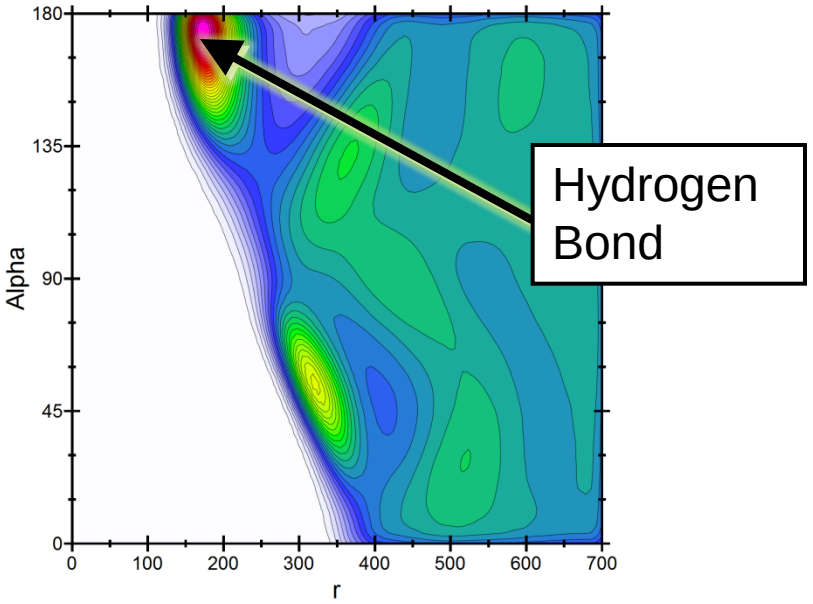

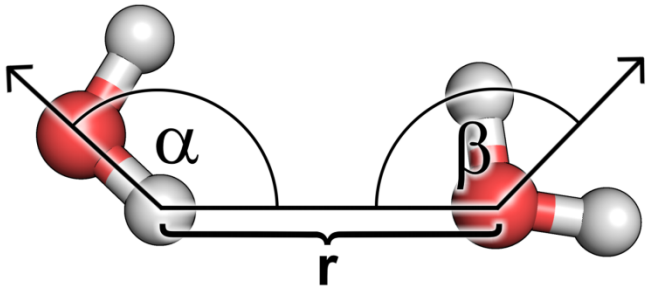

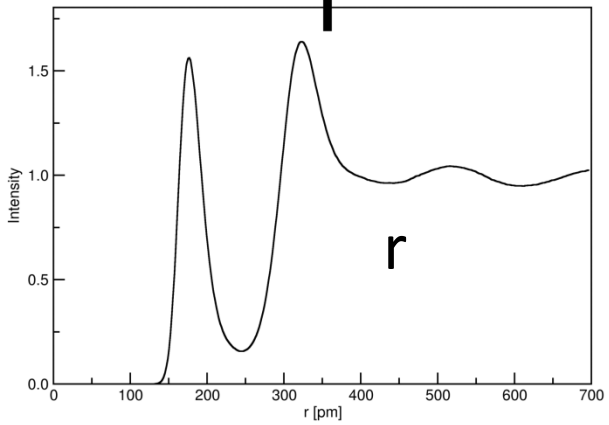

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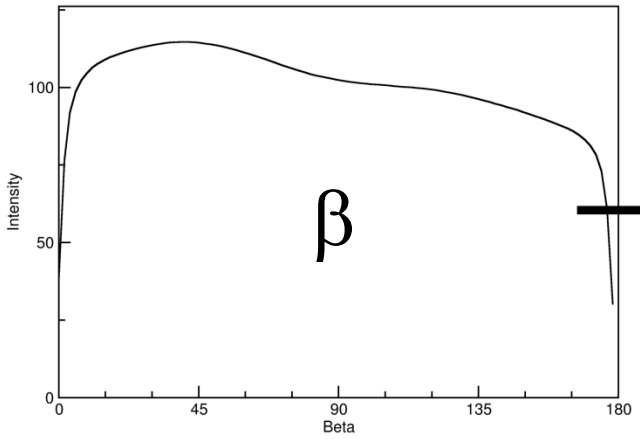

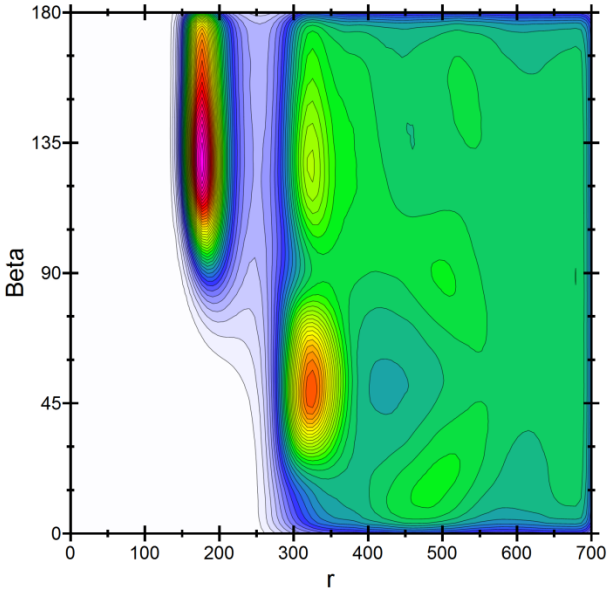

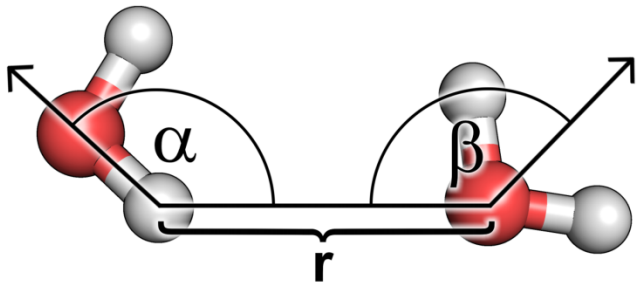

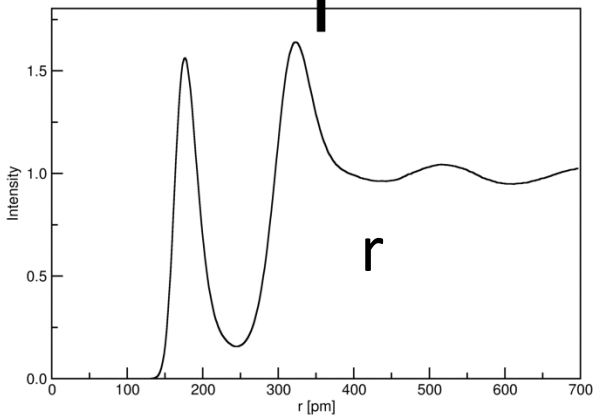

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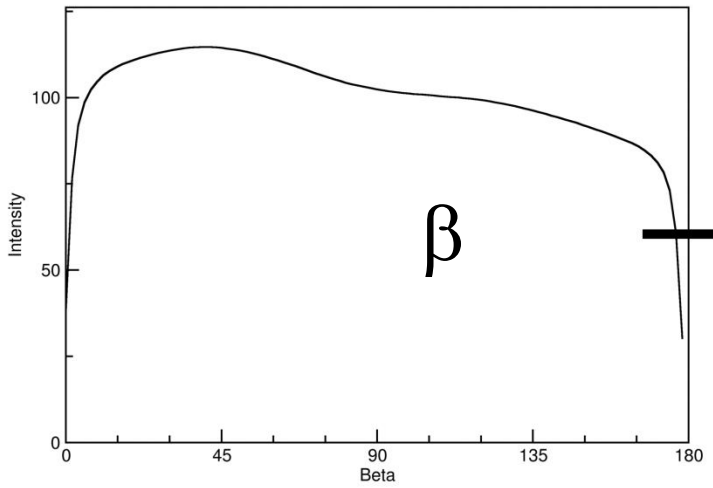
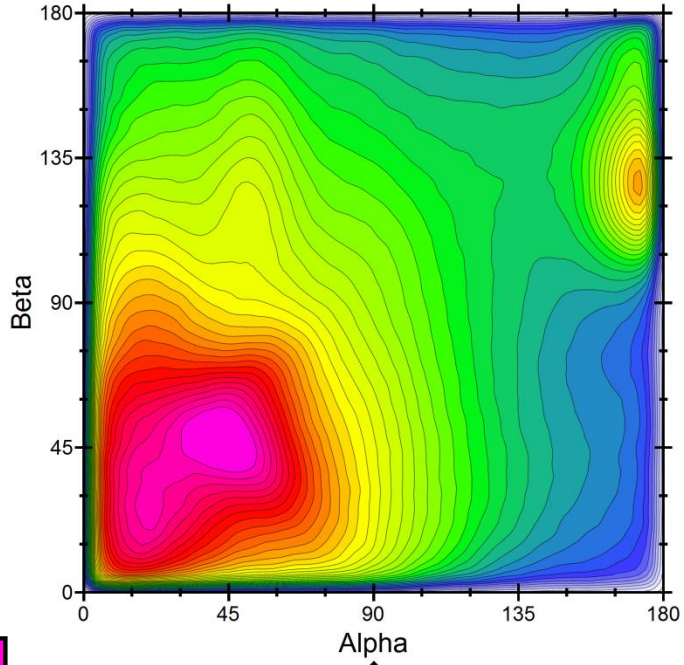
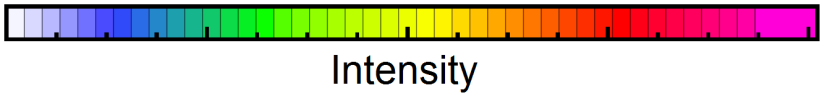
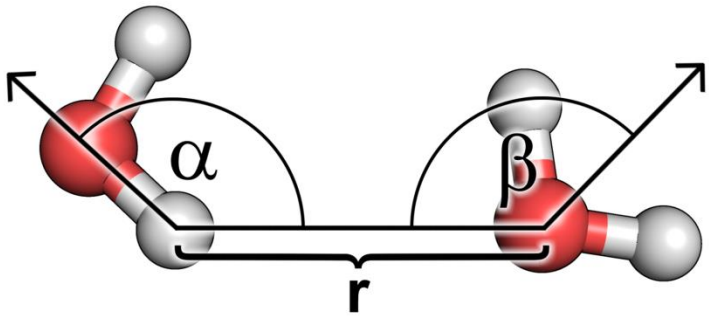
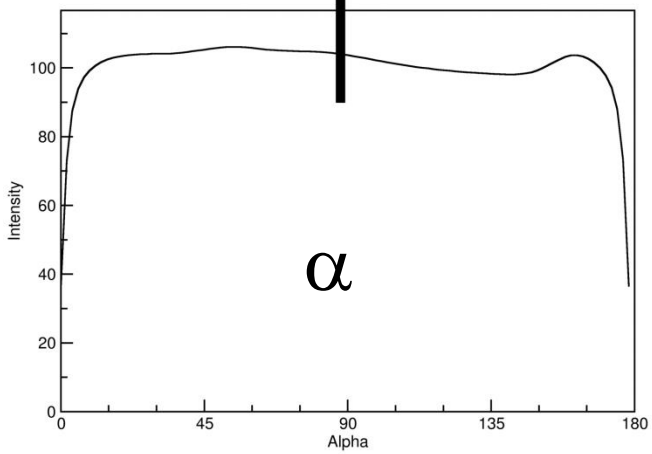






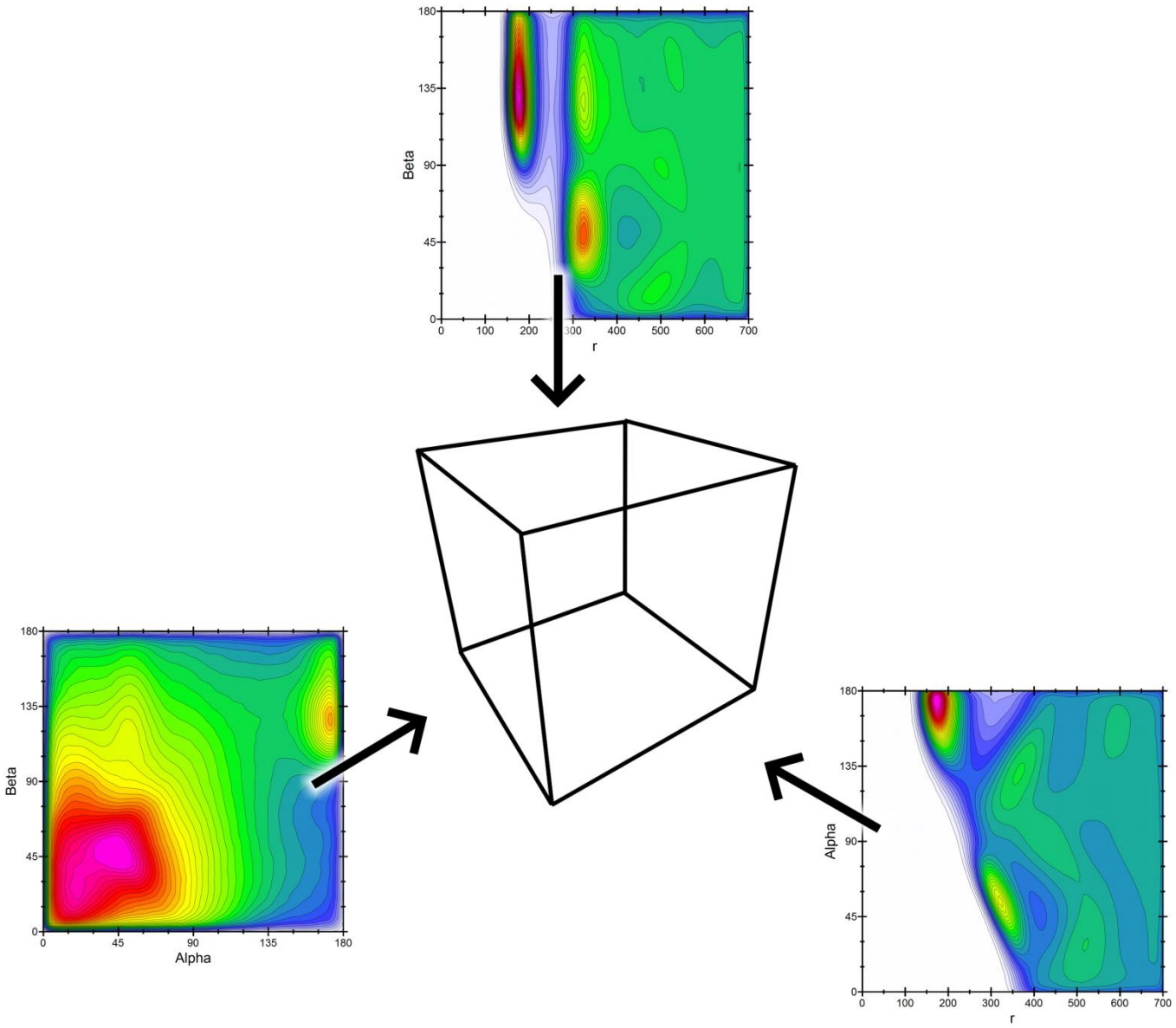




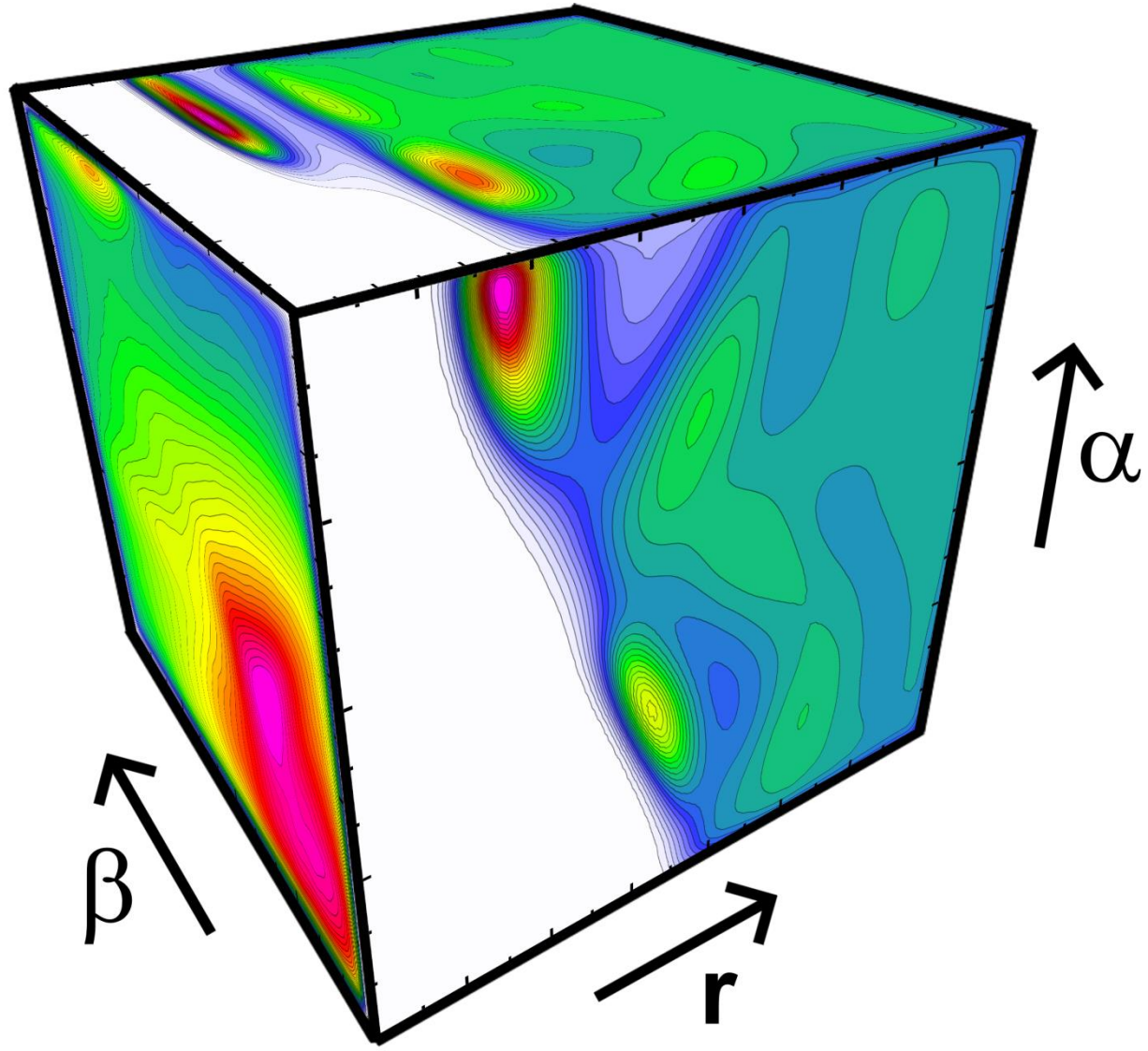
Combined Distribution Functions

- Now we have a 2D distribution
- Much more information can be read out
- What about higher-dimensional histograms? ☺

Combined Distribution Functions



Combined Distribution Functions



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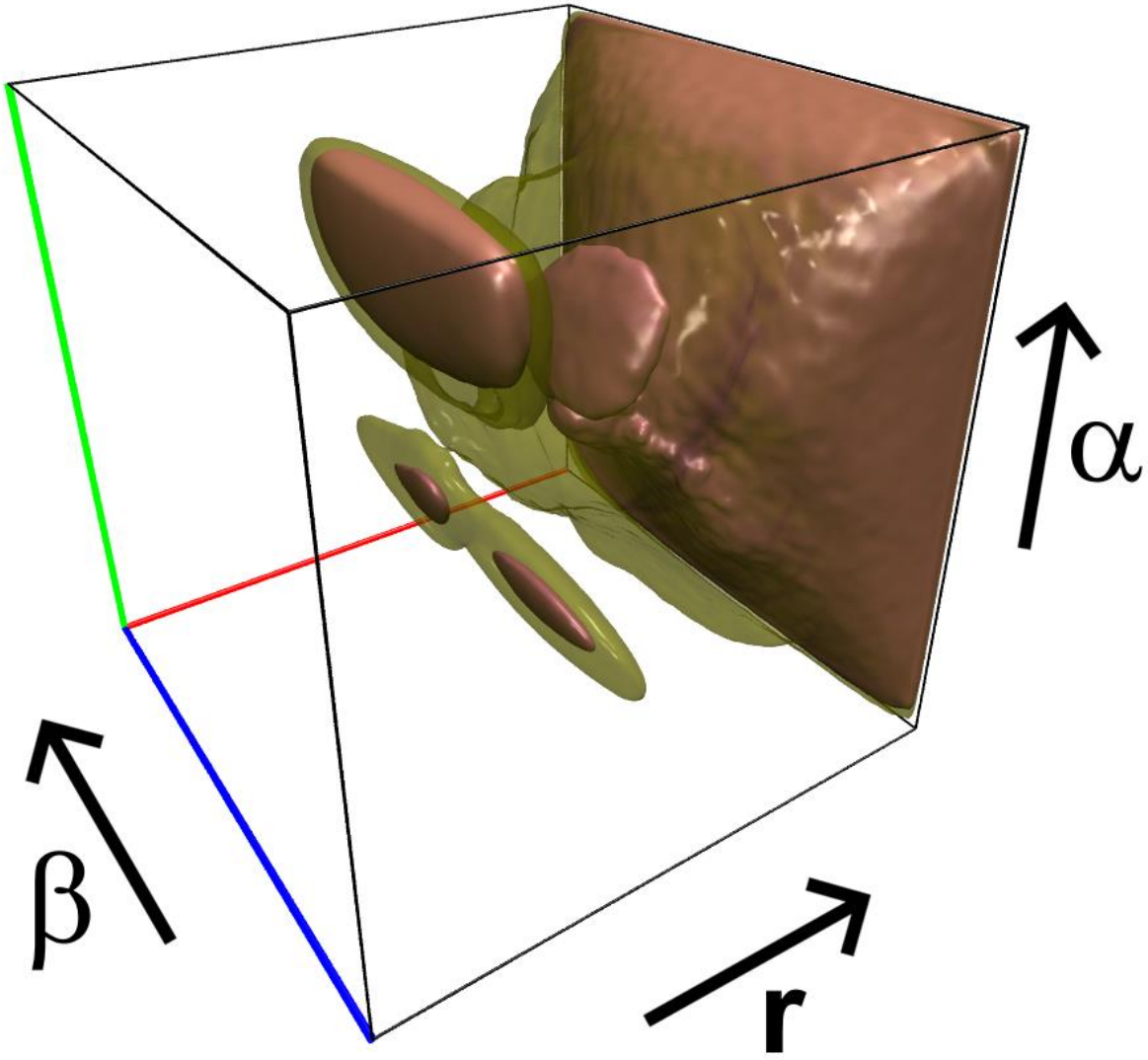

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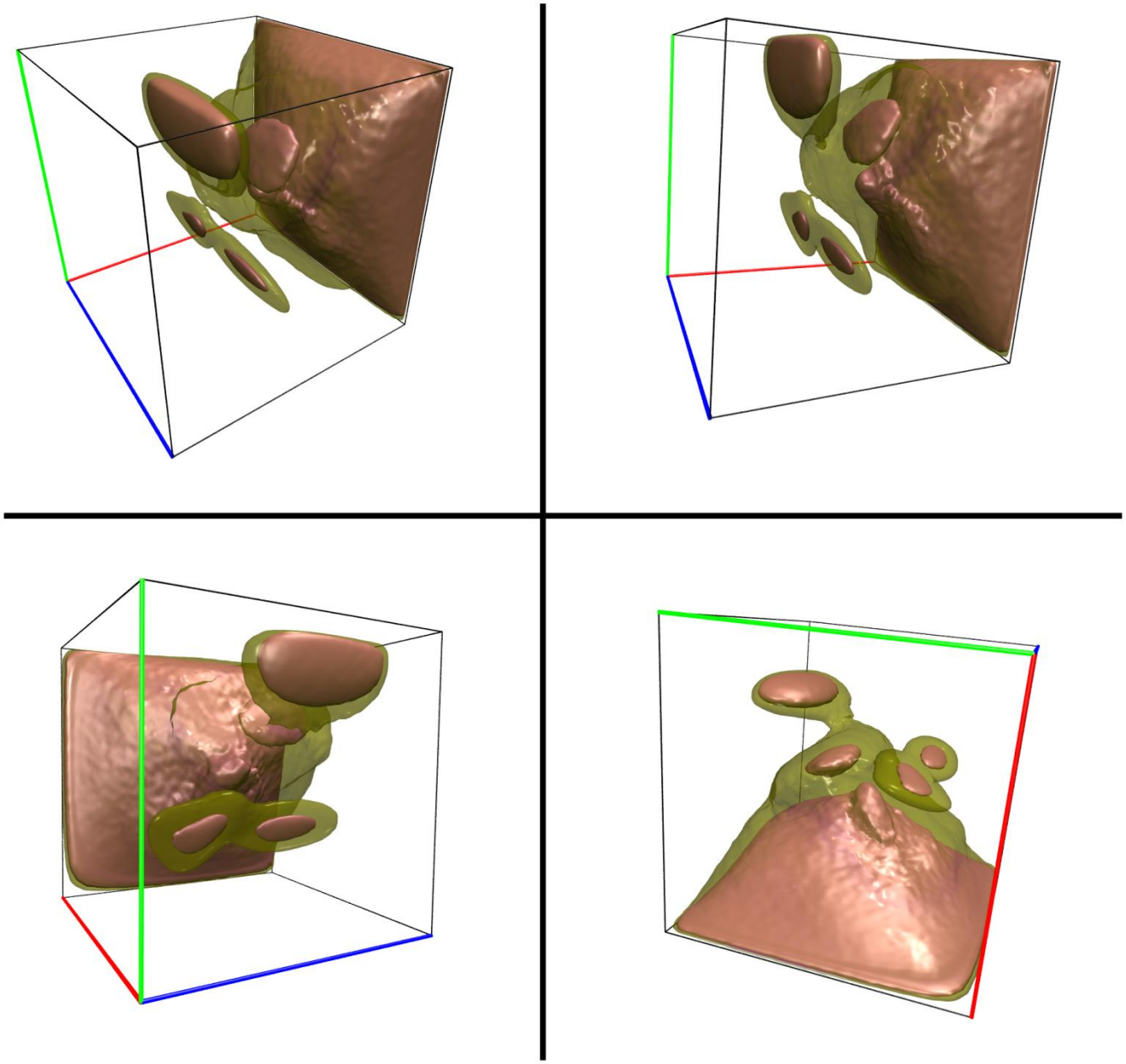


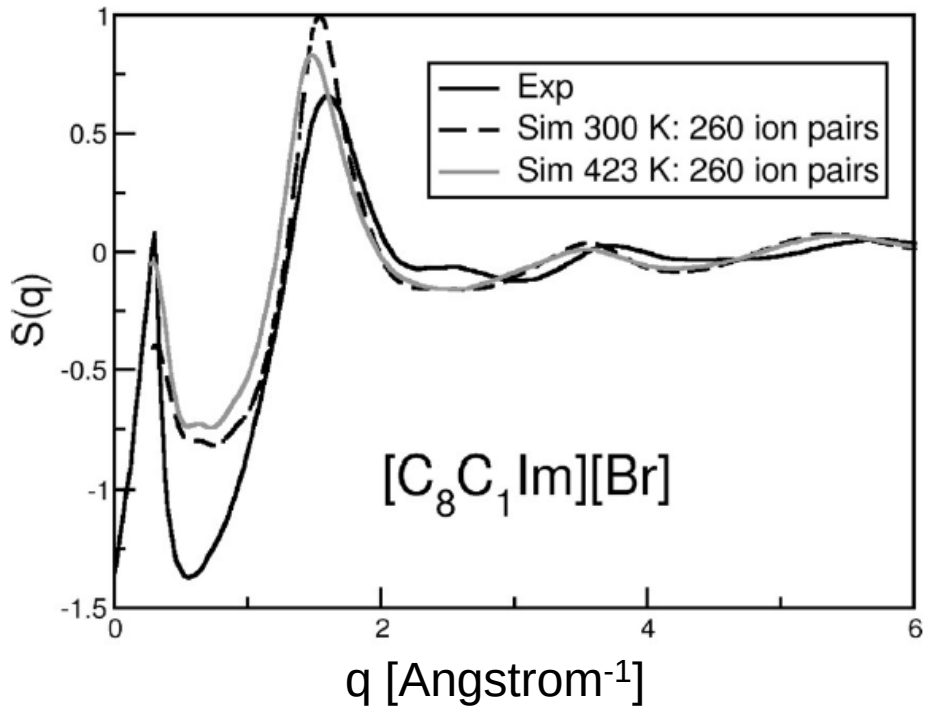
Combined Distribution Functions

- What can be combined?
  - Any distance between two atoms in the system
  - Any angle between three atoms (or two vectors)
  - Any dihedral angle (between 4 atoms or 3 vectors)
  - Absolute velocity of atoms
  - Velocity / force vectors
  - Dipole moments / vectors of molecules

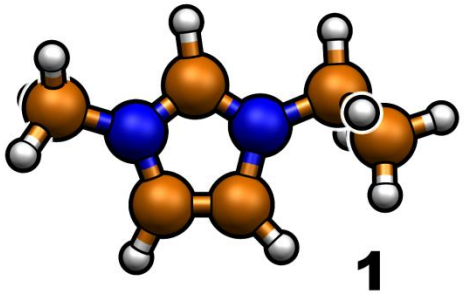
- Combinations can be of any dimensionality
  (shown here only 2D and 3D)

This gives trillions of different combinations!

Structure Factors (Neutron / X ray)



Voronoi Tessellation



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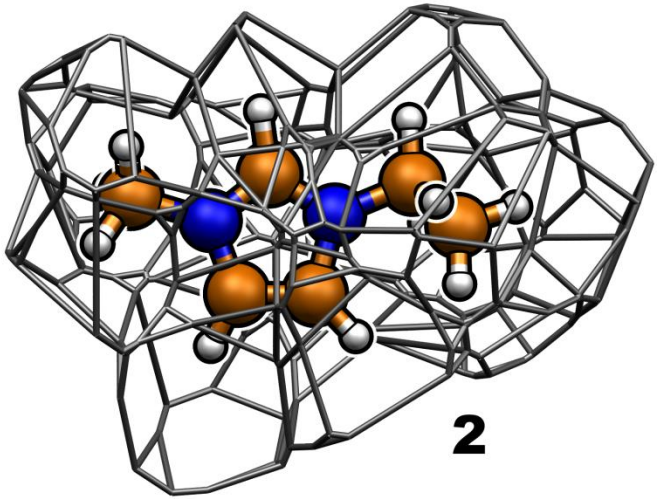

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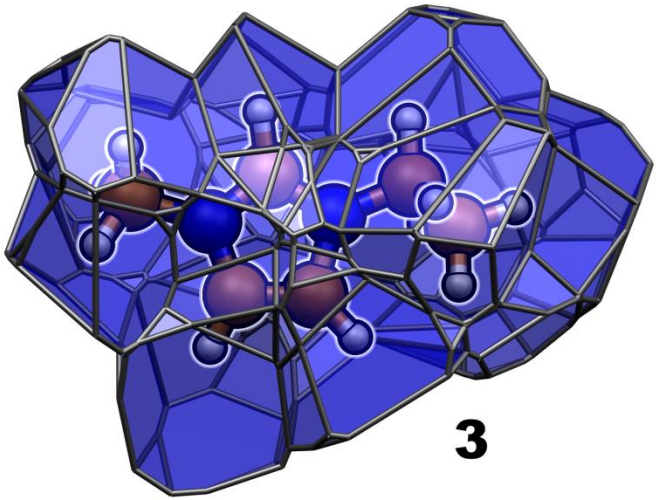

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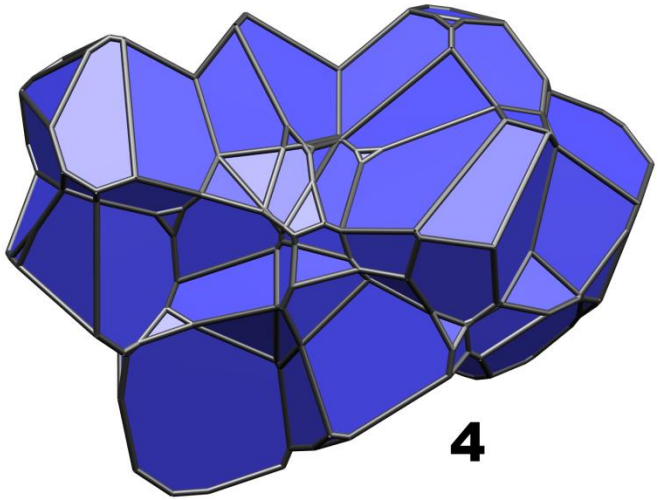
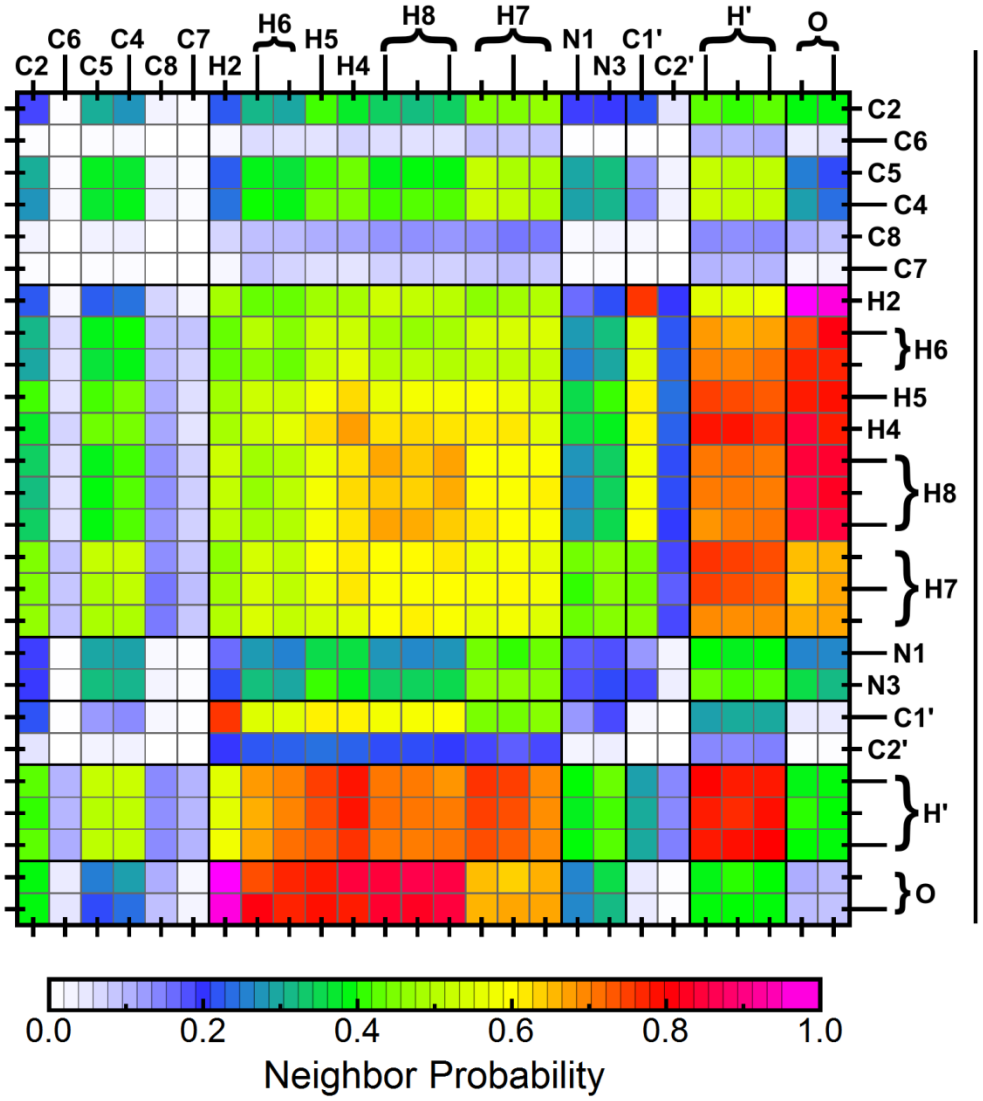
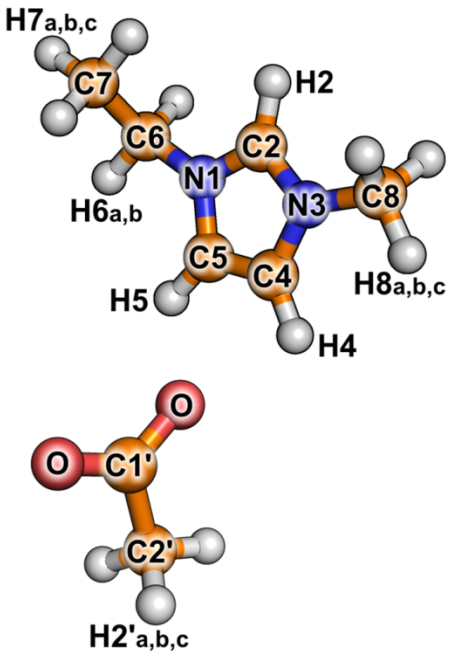


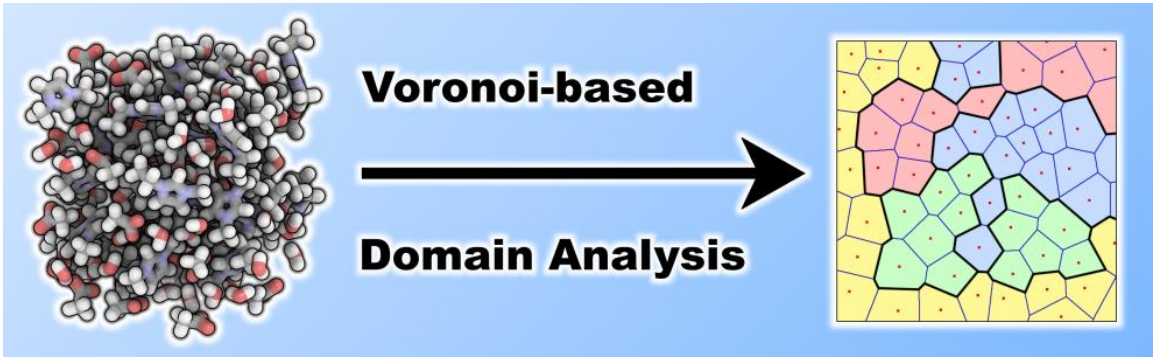
4

Voronoi Neighborhood Analyses

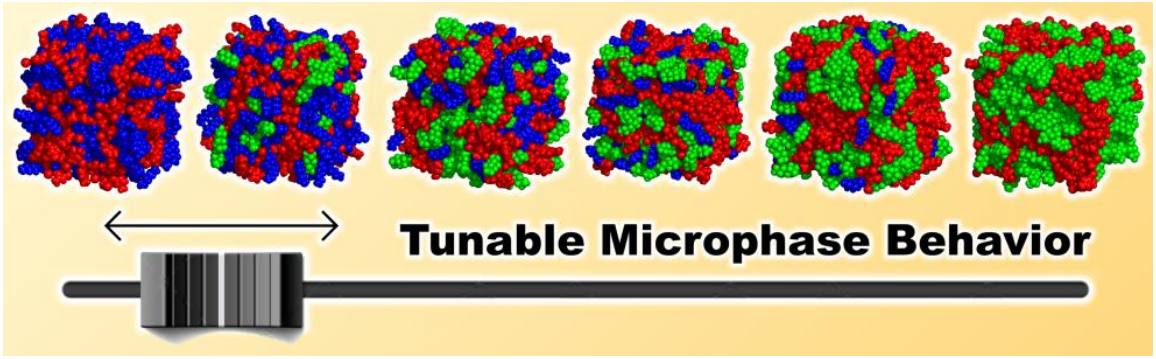




Voronoi-based Domain Analysis

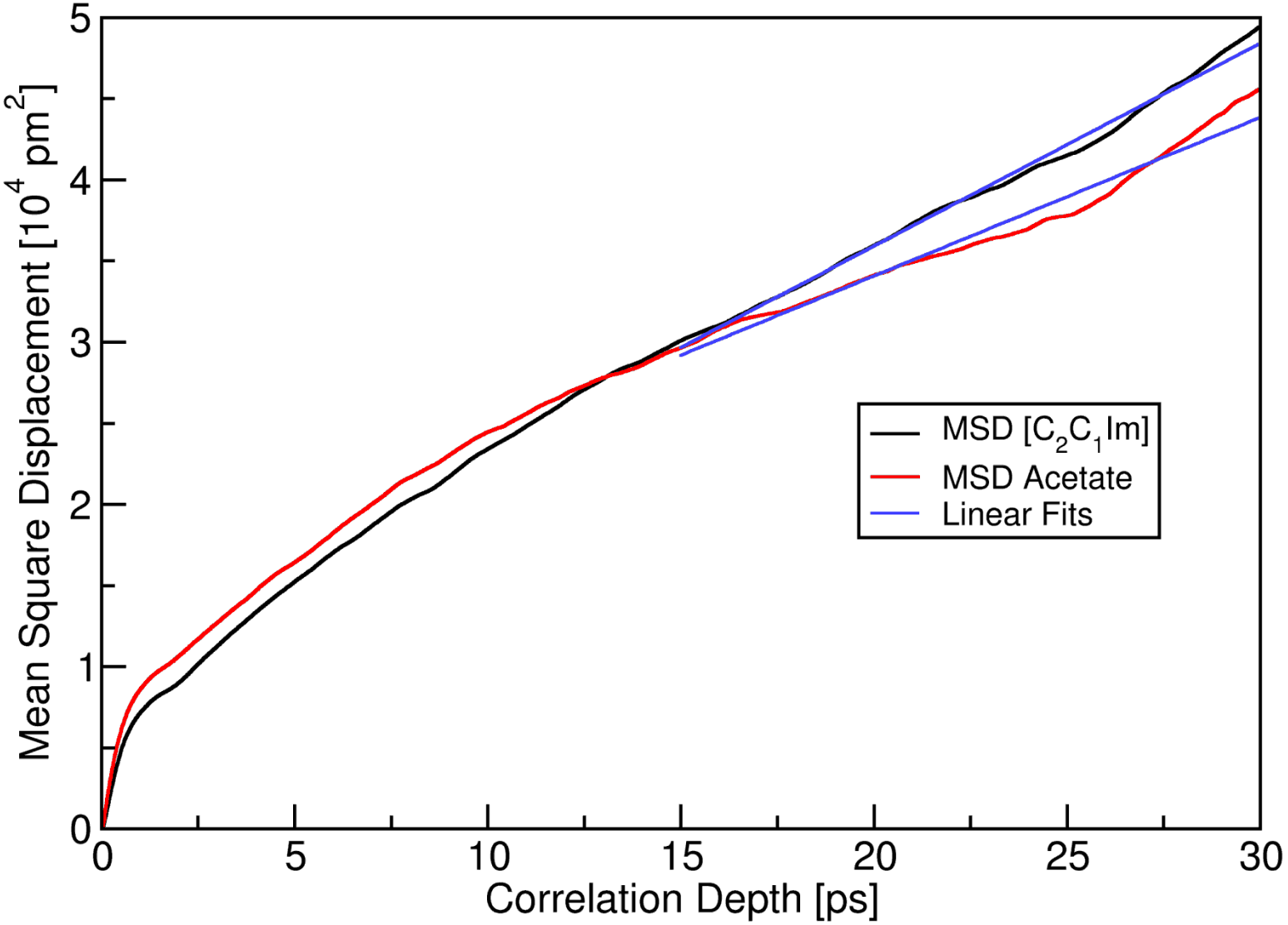


M. Brehm, H. Weber, M. Thomas, O. Holloczki, B. Kirchner: "Domain Analysis in Nanostructured Liquids: A Post-Molecular Dynamics Study at the Example of Ionic Liquids", *ChemPhysChem* **2015**, *16*, 3271–3277.



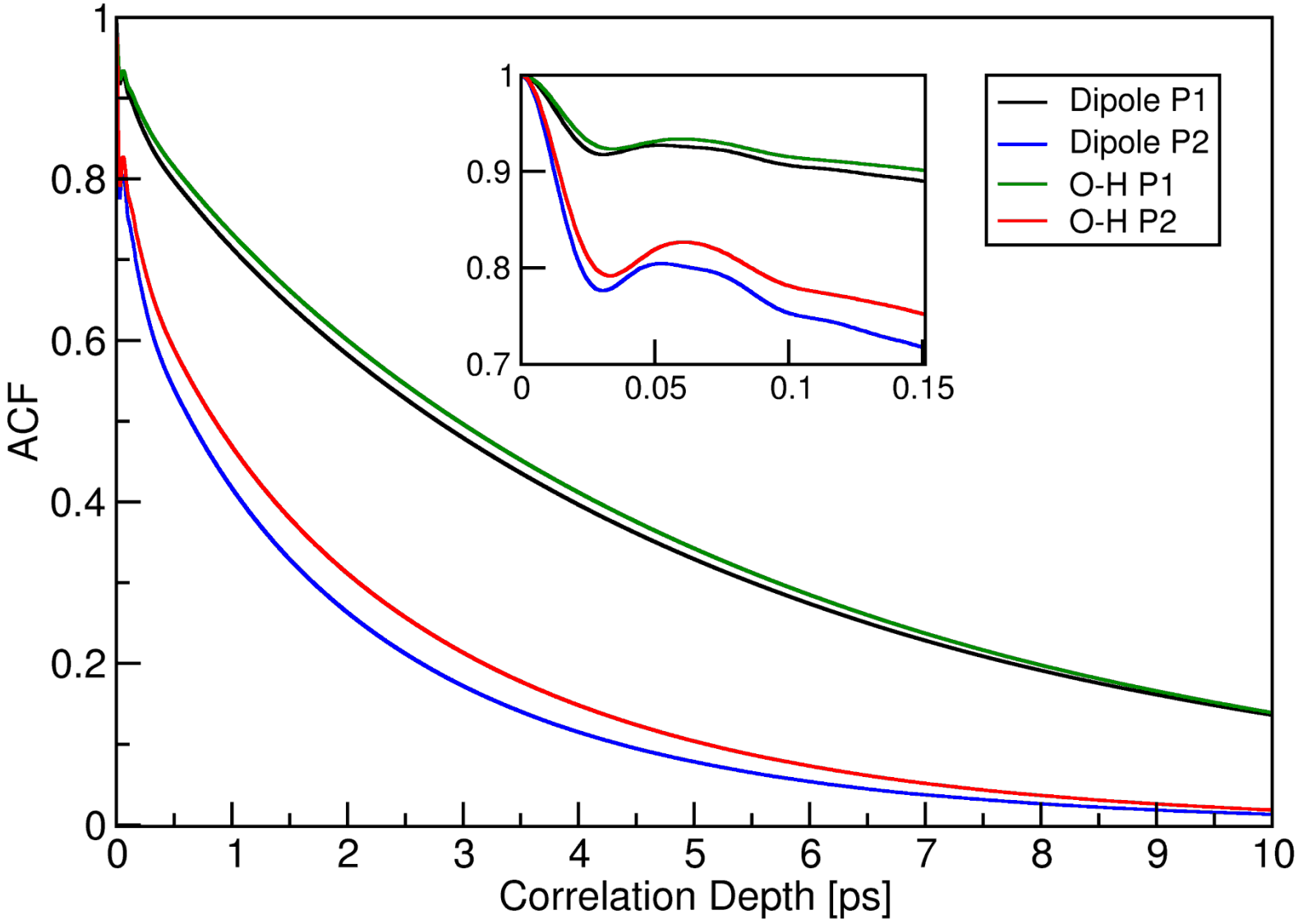
O. Holloczki, M. Macchiagodena, H. Weber, M. Thomas, M. Brehm, A. Stark, O. Russina, A. Triolo, B. Kirchner: "Triphilic Ionic-Liquid Mixtures: Fluorinated and Non-fluorinated Aprotic Ionic-Liquid Mixtures", *ChemPhysChem* **2015**, *16*, 3325–3333.

Dynamical Analyses



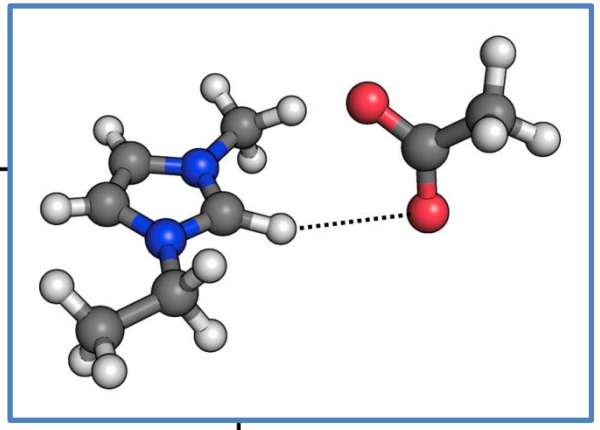
Mean Square Displacement & Diffusion Coefficients

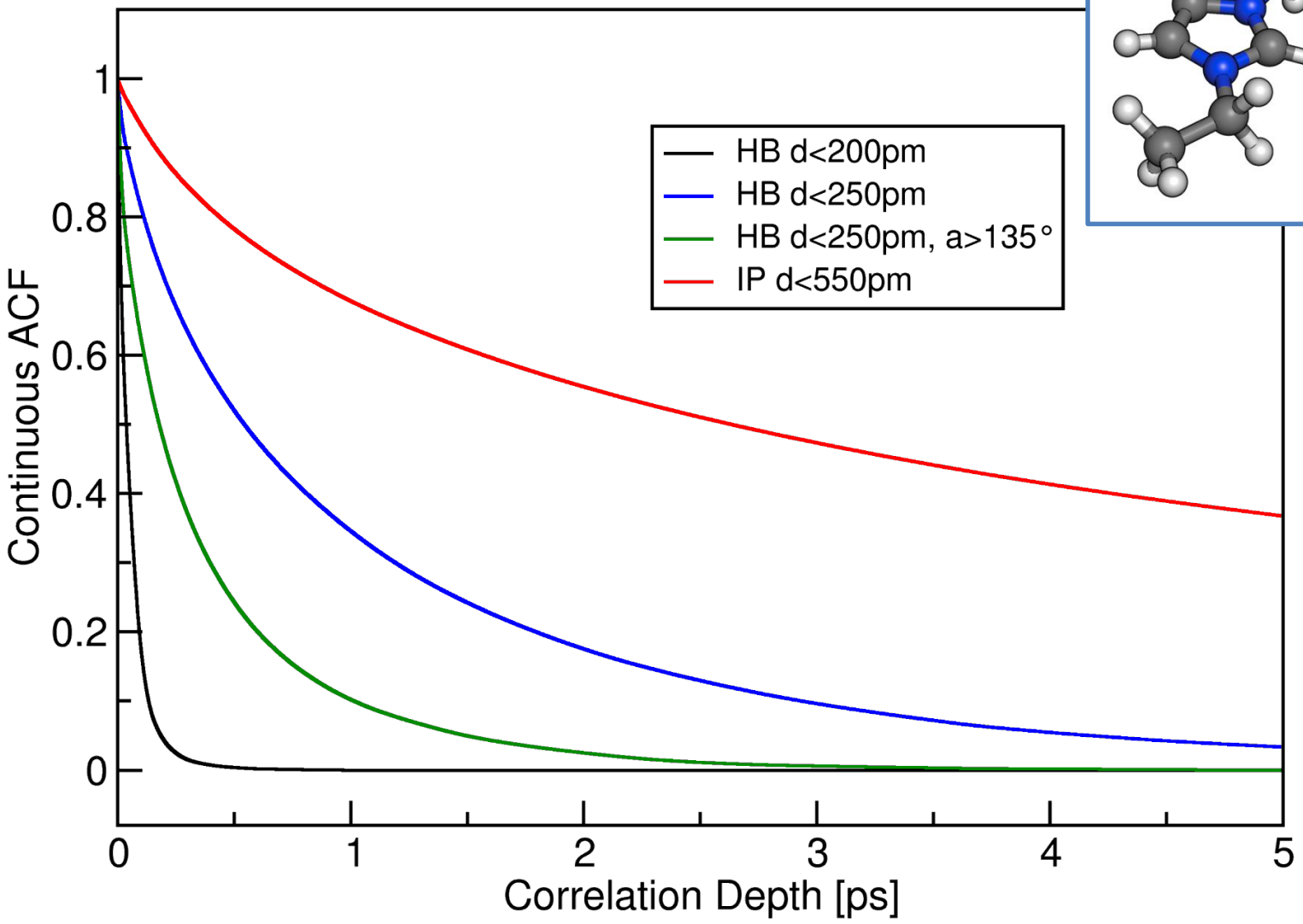
Dynamical Analyses



Vector Reorientation Dynamics

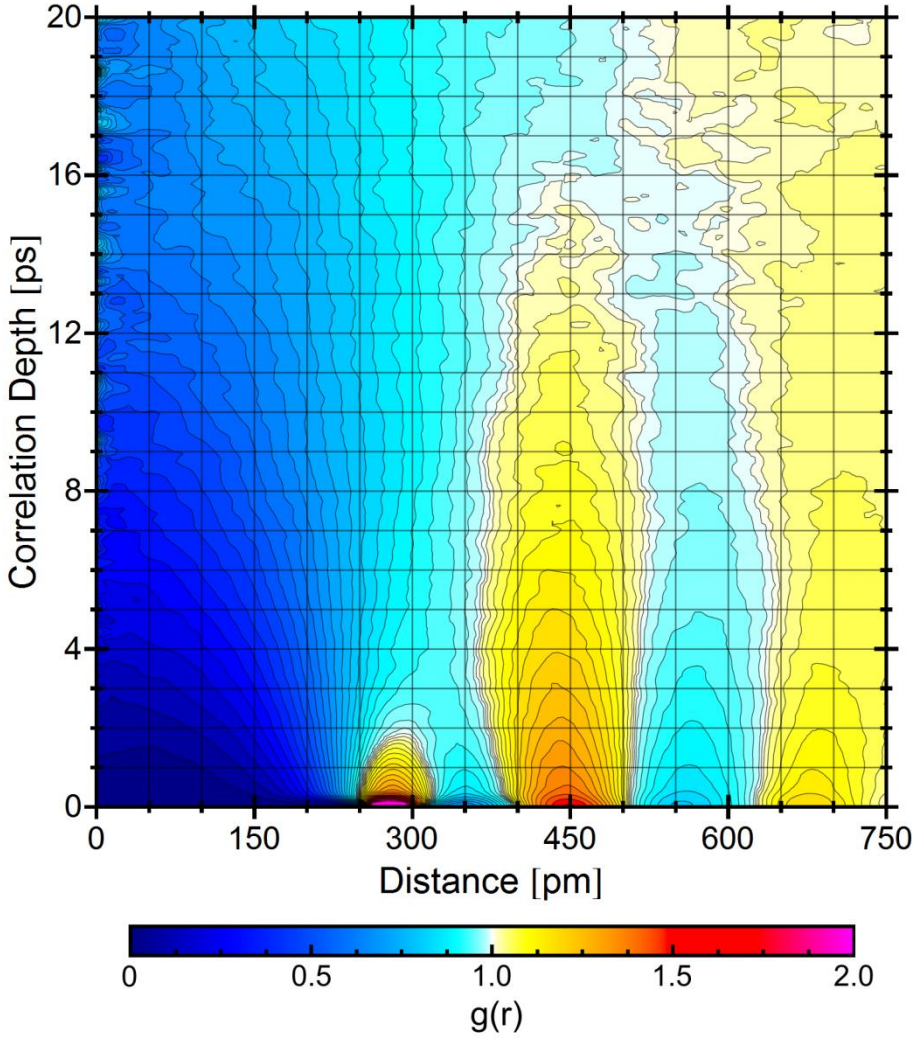
Dynamical Analyses





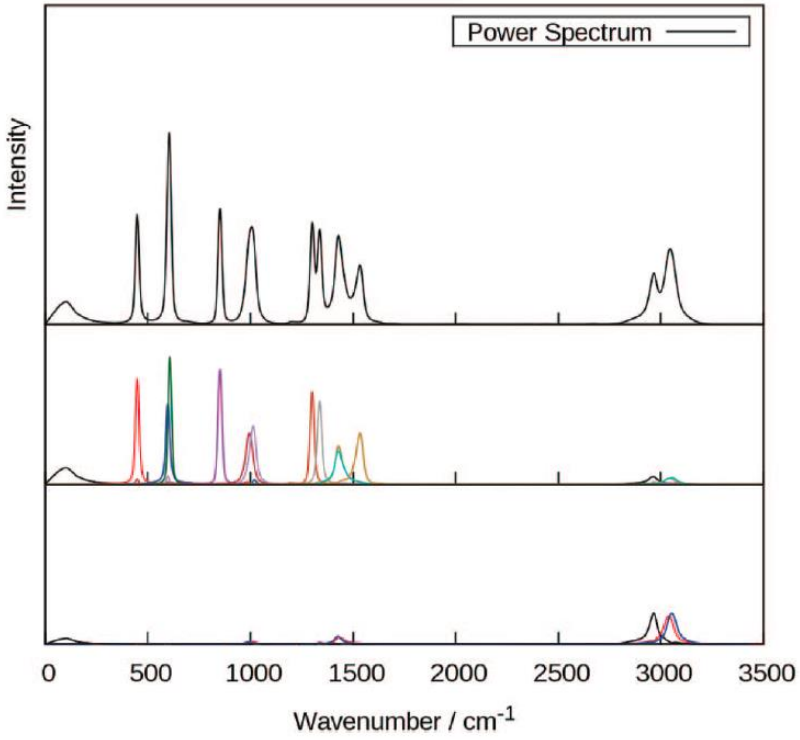
Lifetime of Aggregates (e.g., hydrogen bonds)

Dynamical Analyses

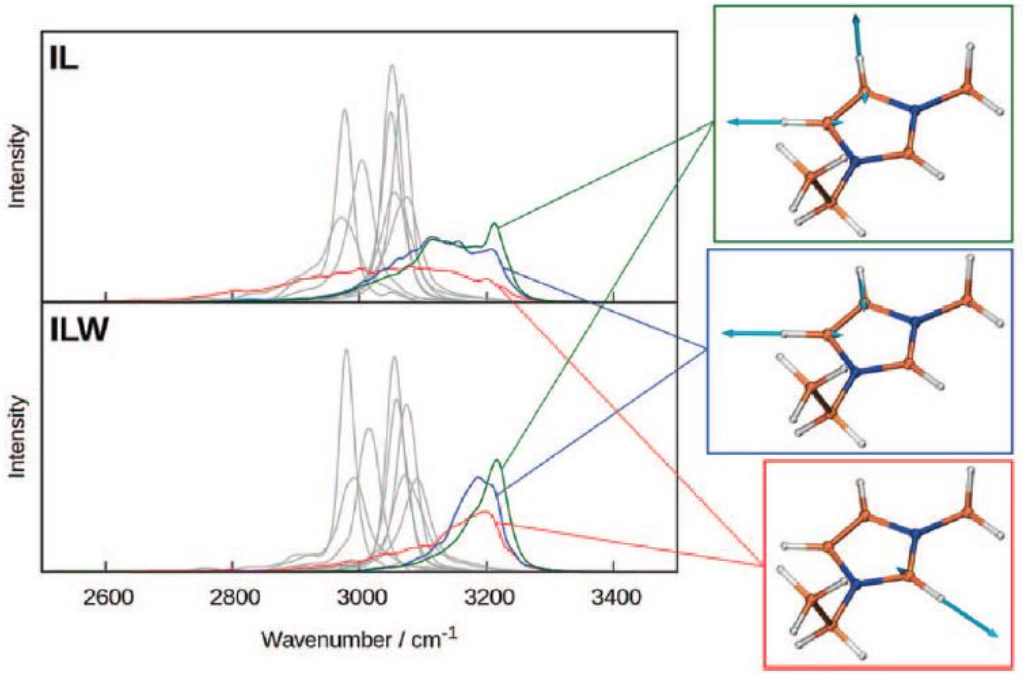


Van Howe Correlation Function & Dynamic Structure Factor

Spectroscopic Analyses



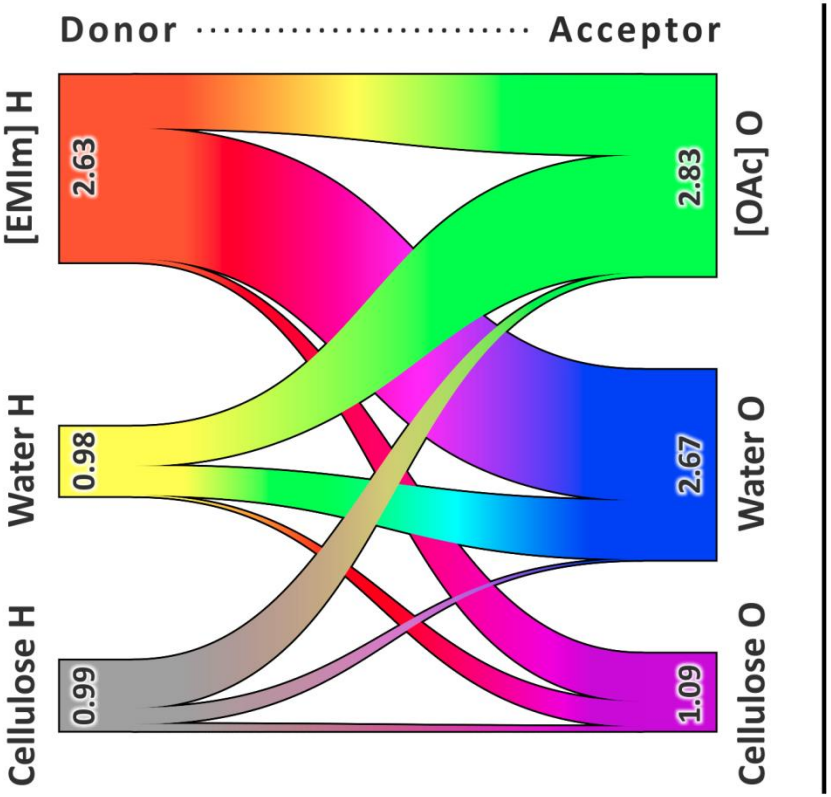
Normal Modes from bulk phase AIMD

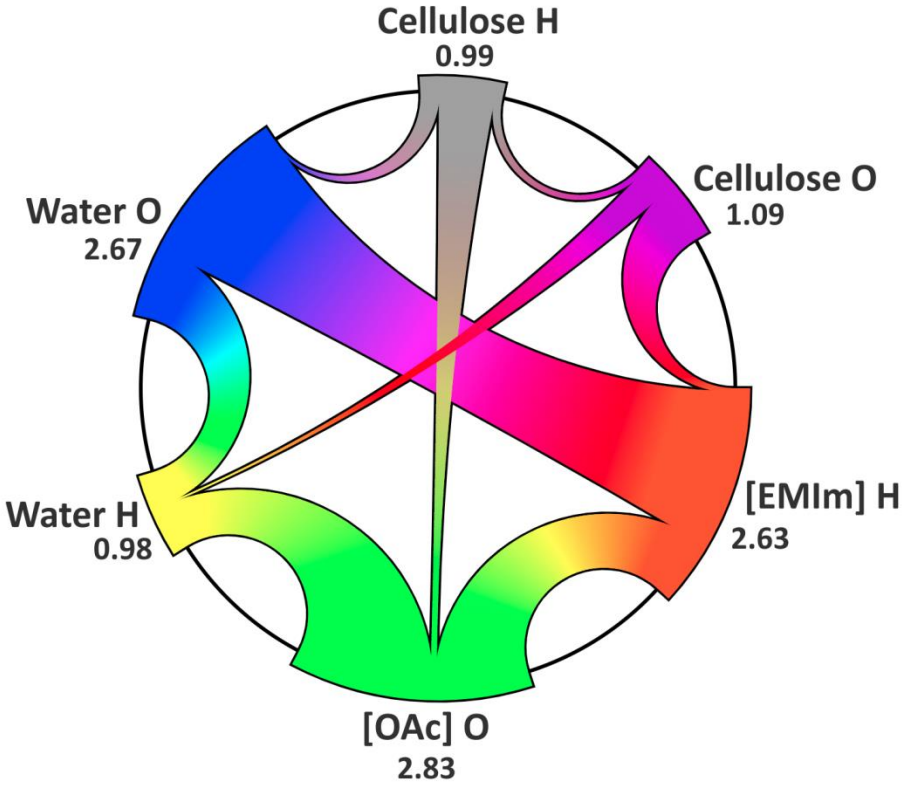


M. Thomas, M. Brehm, O. Holloczki,
Z. Kelemen, L. Nyulaszi, T. Pasinszki, B. Kirchner,
J. Chem. Phys. **2014**, *141*, 024510.

Hydrogen Bond Topology

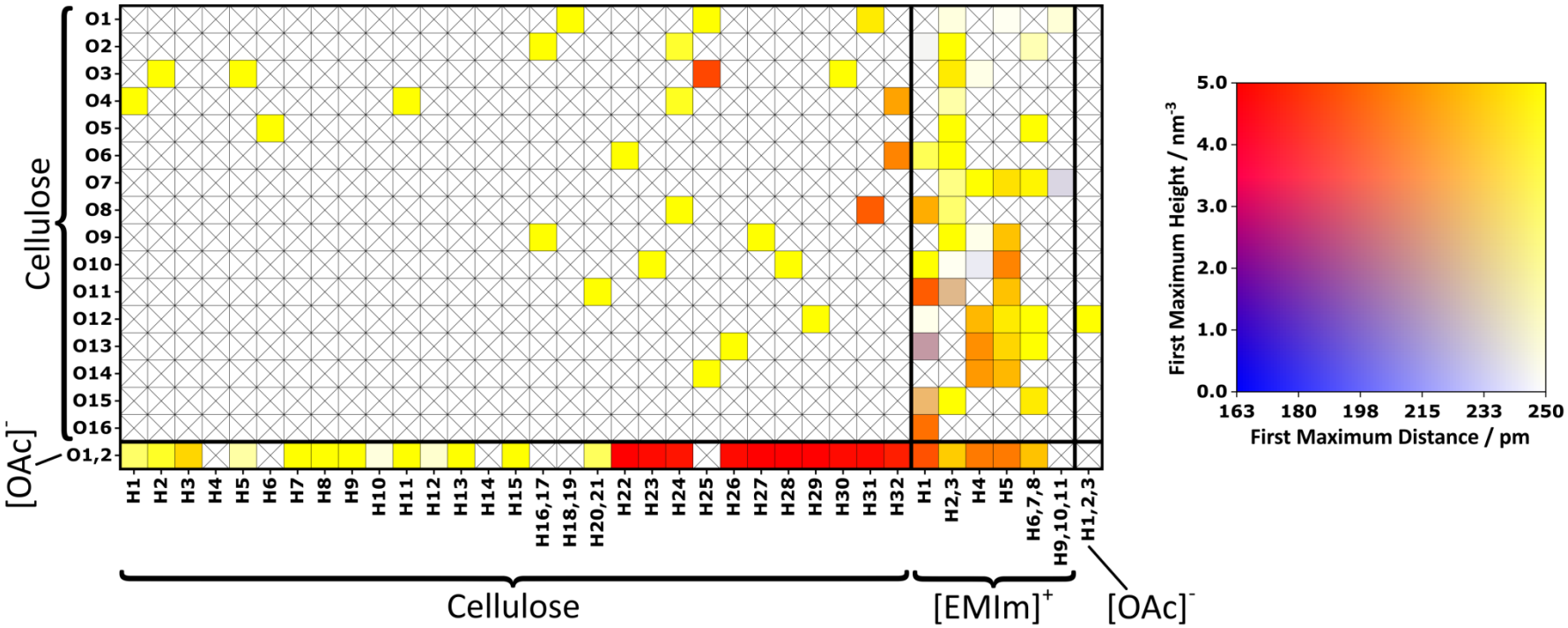
Sankey Diagrams





Hydrogen Bond Topology

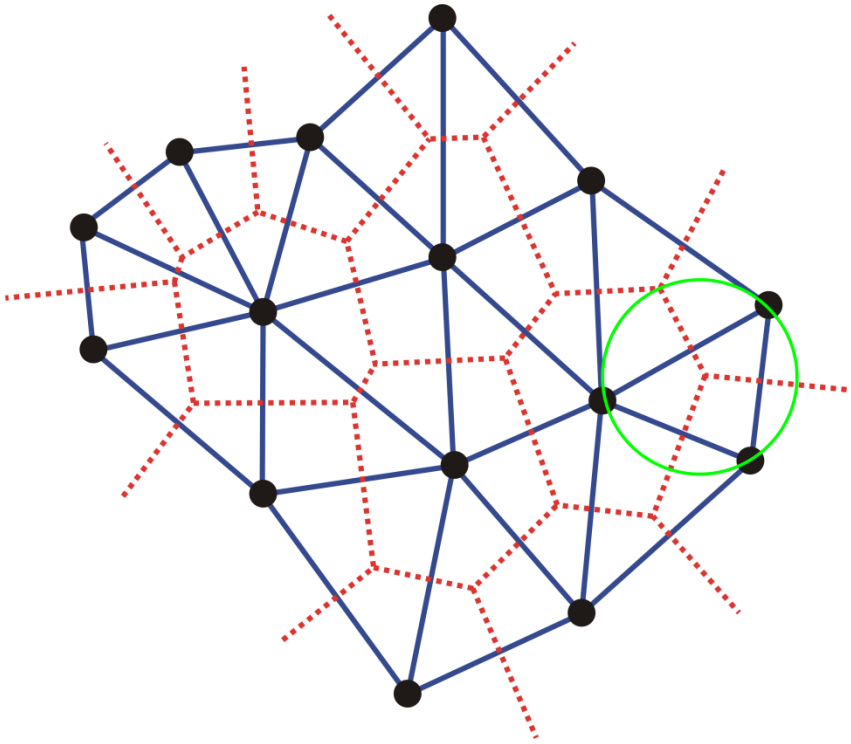
Connection Matrix Analysis

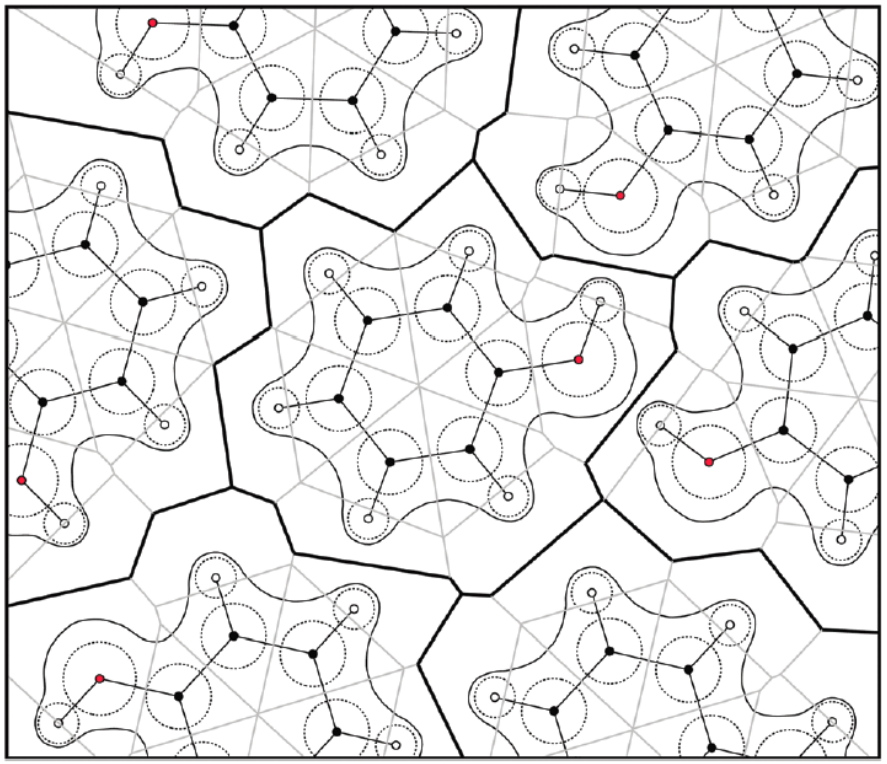


3.) Voronoi Charges

Voronoi Charges

Voronoi Tessellation (G. Voronoi, 1908):





→ Can be used to compute atomic partial charges
by simply integrating the total electron density in Voronoi cells

M. Brehm, M. Thomas, *Molecules* **2021**, *26 (7)*, 1875.

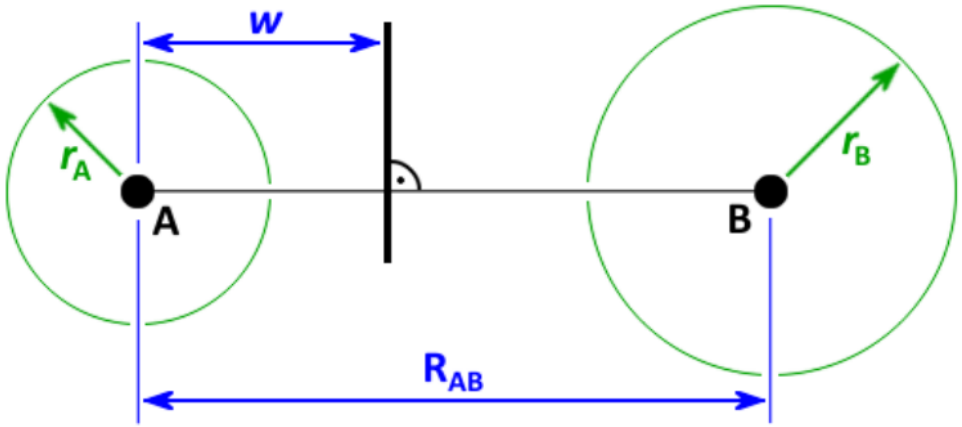
Voronoi Charges

Problem: Atom radii not taken into account

→ Hydrogen atoms are assigned too much electron density

Possible solution: **„Radical Voronoi tessellation“**

Atoms now have radii which determine the size of their Voronoi cell



$$w := \left(\frac{1}{2} + \frac{r_A^2 - r_B^2}{2R_{AB}^2}\right) R_{AB}$$

M. Brehm, M. Thomas, *Molecules* **2021**, *26 (7)*, 1875.

Voronoi Charges

Subsequent Problem: Empirical parameters → no longer unbiased

Which atom radii to use? Covalent? VdW?

Our idea: In molecular liquids, charge transfer between molecules should not be significant...

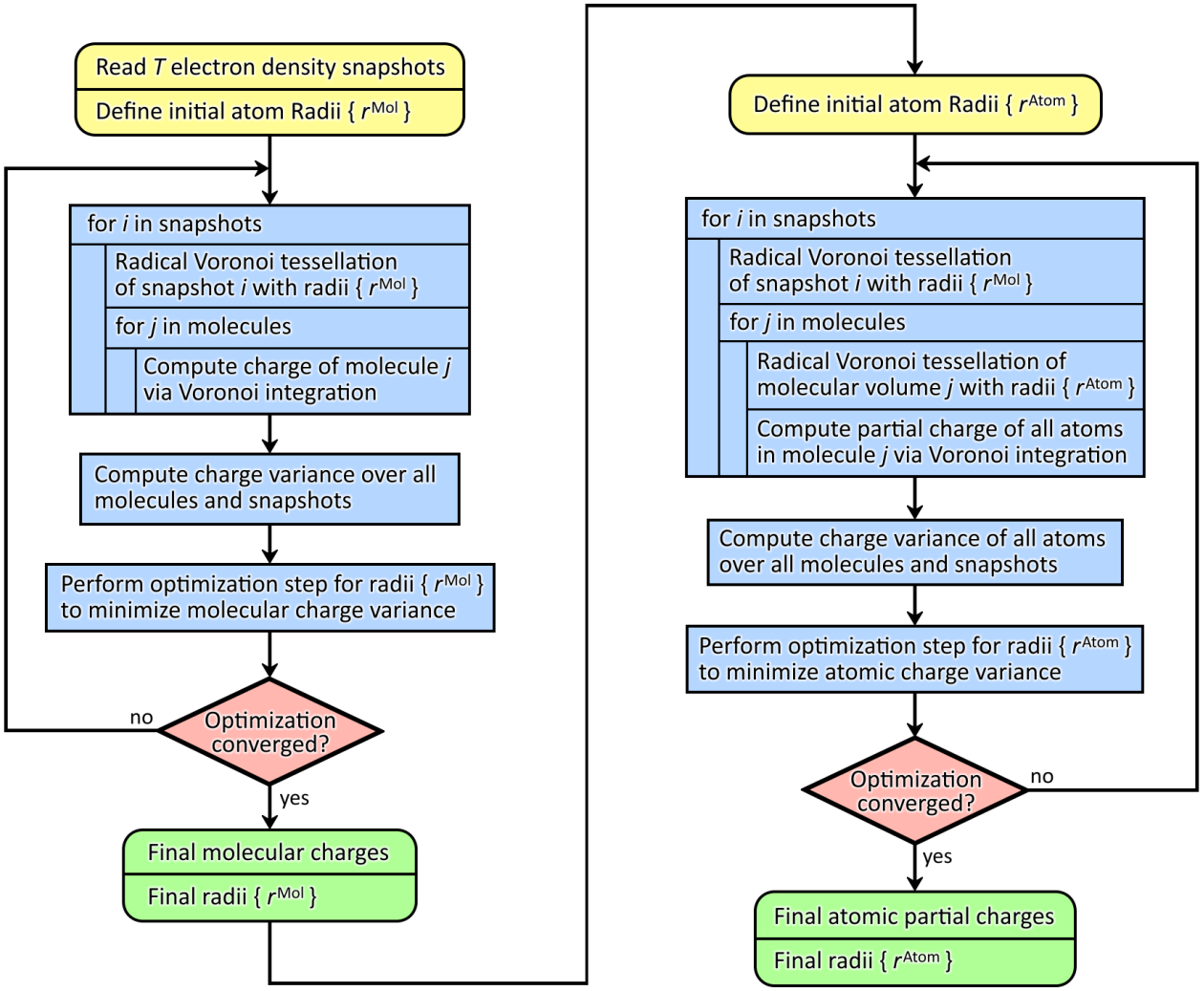
→ Optimize the Voronoi radii so that the „fluctuation“ (variance) of the atomic charges becomes minimal!

Obtain a set of optimized atom radii and atom charges
for a particular trajectory *(dependent on temperature, pressure, ...)*

Very well suitable for „dense“ bulk phase systems.

M. Brehm, M. Thomas, *Molecules* **2021**, *26 (7)*, 1875.

Voronoi Charges

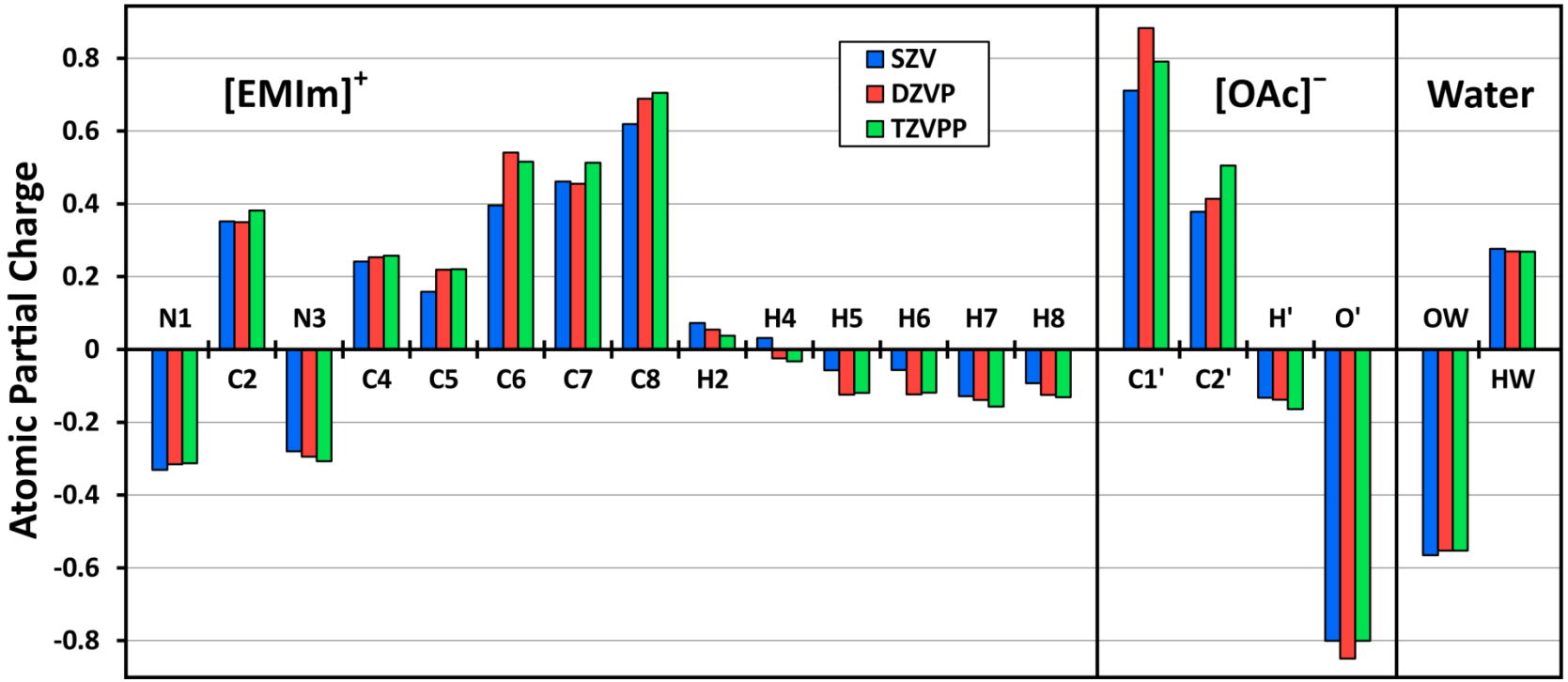


(a) Molecular Optimization ***(b) Atomic Optimization***

M. Brehm, M. Thomas, *Molecules* **2021**, *26 (7)*, 1875.

Voronoi Charges

Very small basis set dependency:



M. Brehm, M. Thomas, *Molecules* **2021**, *26 (7)*, 1875.

Voronoi Charges

Interesting effects are automatically captured:

- Ion charges smaller than unity (+/- 0.8) in ionic liquids *(often applied empirically before)*
- Polarization of the cation and depolarization of the anion in ionic liquids when water is added *(observed before)*

Conclusions:

- New approach to obtain atomic point charges
- No empirical parameters; optimized radii come out as by-product
- Well suitable for periodic bulk phase systems
- Very small basis set dependence
- Requires only total electron density → works with many methods

M. Brehm, M. Thomas, *Molecules* **2021**, *26 (7)*, 1875.

Voronoi Charges

Published in 2021:

M. Brehm, M. Thomas, *Molecules* **2021**, *26 (7)*, 1875.

Open Access Article

Optimized Atomic Partial Charges and Radii Defined by Radical Voronoi Tessellation of Bulk Phase Simulations

by Martin Brehm * and Martin Thomas

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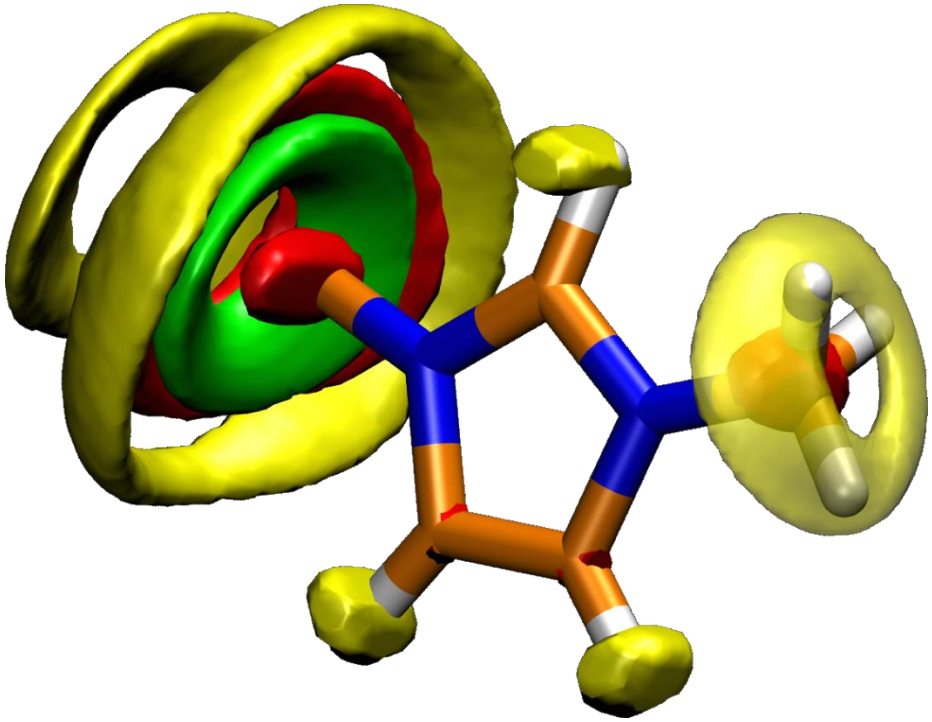
Abstract

We present a novel method for the computation of well-defined optimized atomic partial charges and radii from the total electron density. Our method is based on a two-step radical Voronoi tessellation of the (possibly periodic) system and subsequent integration of the total electron density within each Voronoi cell. First, the total electron density is partitioned into the contributions of each molecule, and subsequently the electron density within each molecule is assigned to the individual atoms using a second set of atomic radii for the radical Voronoi tessellation. The radii are optimized on-the-fly to minimize the



Thank you for your attention!