Milano Chemistry Molecular Simulation (MiCMoS):
a versatile tool to study molecular systems in condensed phase

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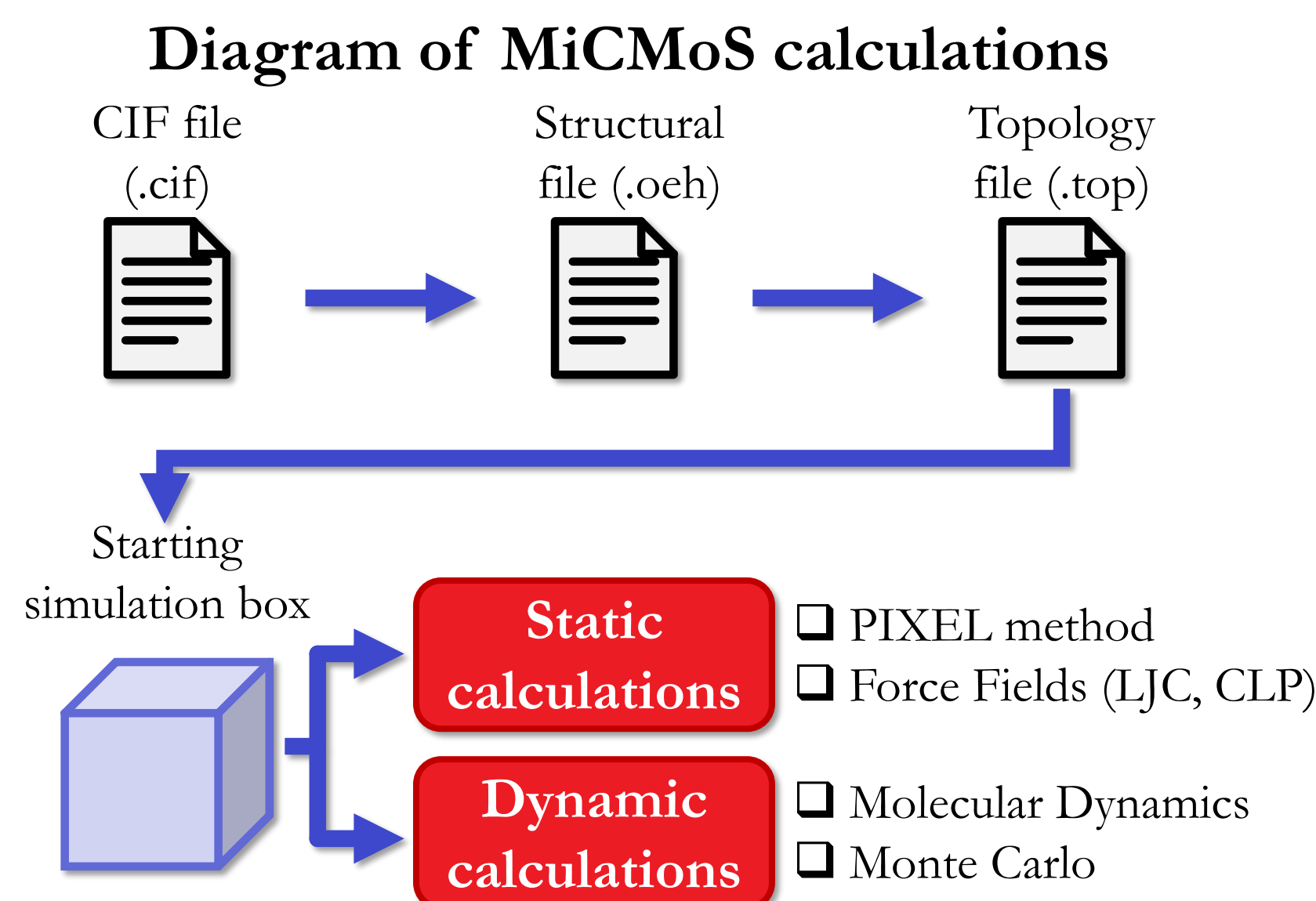[2]Istituto Nazionale di Fisica Nucleare (INFN), Laboratori Nazionali di Frascati, Frascati (Italy)
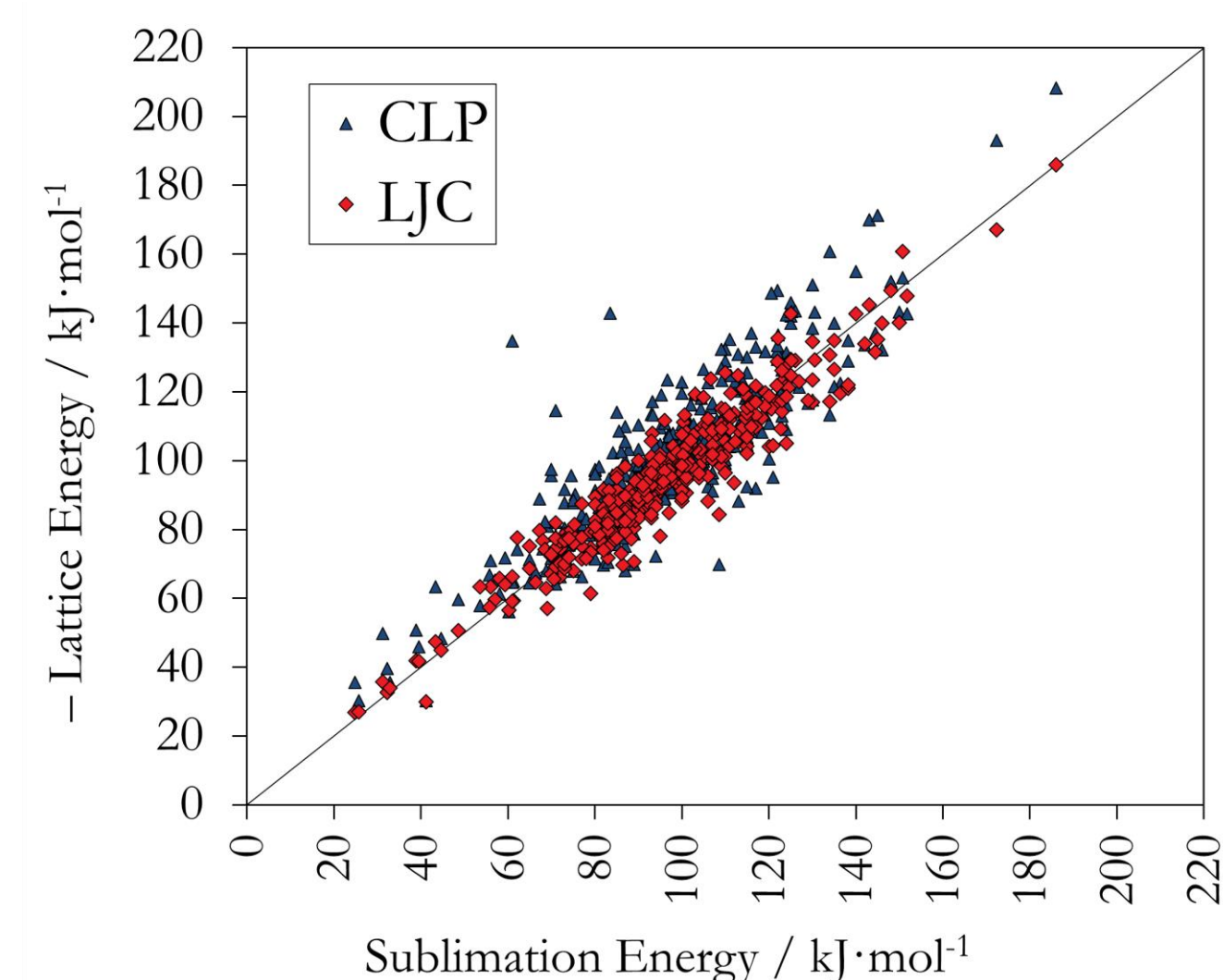
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INTRODUCTION

The Milano Chemistry Molecular Simulation (**MiCMoS**) platform is a powerful computational tool, specifically designed to study **molecular systems** in condensed phase[1,2]. The software offers a wide range of capabilities and is freely available to the scientific community, together with step-by-step tutorials. Within a matter of minutes, MiCMoS allows to generate input files for both static and dynamic calculations (**Molecular Dynamics** and **Monte Carlo**), and has two force fields, LJC and CLP, both accurately calibrated against sublimation and vaporization enthalpies[3].

Diagram of MiCMoS calculations

CIF file (.cif) → Structural file (.oeh) → Topology file (.top)

Starting simulation box

Static calculations
☐ PIXEL method
☐ Force Fields (LJC, CLP)

Dynamic calculations
☐ Molecular Dynamics
☐ Monte Carlo

**Calibration of the Force Fields**

RESULTS

MiCMoS offers the PIXEL module to accurately calculate interaction energies with a 100-fold reduction in computational time compared to ab initio methods. In addition, the static picture is complemented by Molecular Dynamics simulations, which provide insights into the system's dynamics, and Monte Carlo simulations, which are highly valuable for studying equilibrium properties.
Here, a few examples of MiCMoS capabilities are reported, extracted from the following broad areas:

1. Determination of **interaction energies**
2. MD simulation of **bulk crystals**
3. MD simulation of **isolated nanocrystals**
4. MD simulation of **liquids** in **confined spaces**
5. Study and analysis of **molecular aggregation**

### 1. Interaction energies of halogen bonds with PIXEL
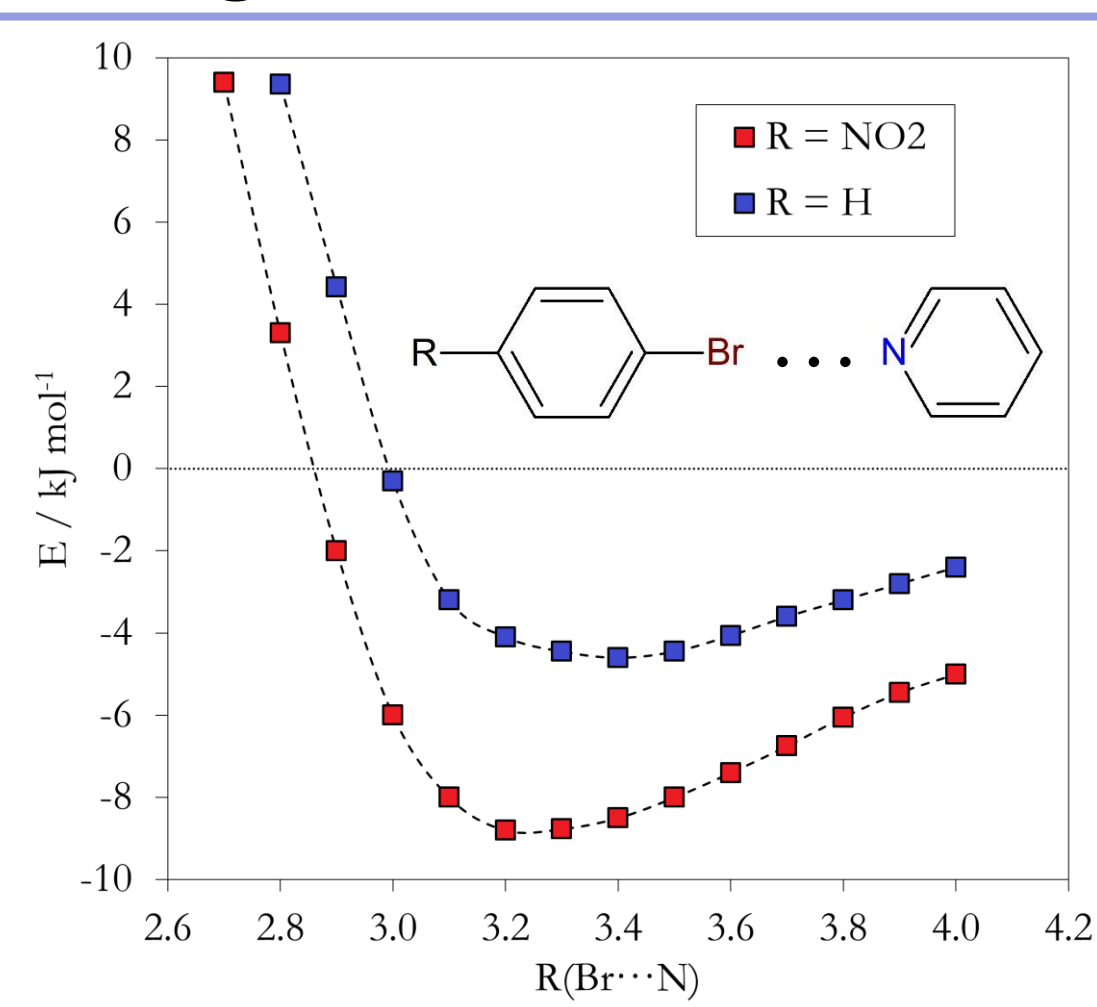
The N···Br halogen bond energy between pyridine and bromobenzene increases from 4 to 9 kJ mol^{-1} with the nitro substitution, still less than half of the energy of weak alcohol H-bonds (25 kJ mol^{-1})[4].

2. Study of crystalline and plastic phases

1,4-cyclohexadiene

153 K — Crystalline phase
300 K — Plastic phase
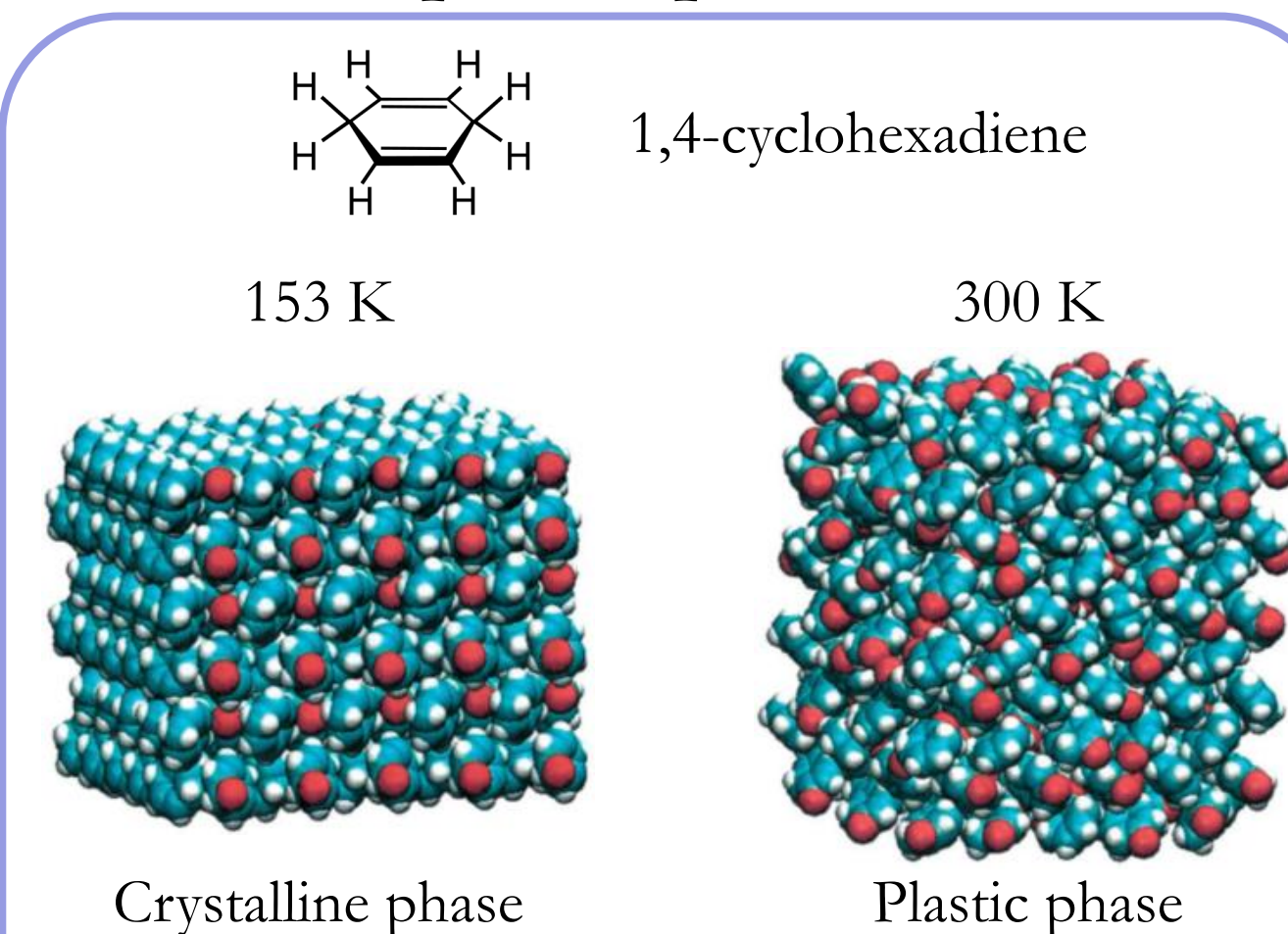
At high T, 1,4-cyclohexadiene crystal shows a quick loss of rotational correlation while keeping the distribution of centers of mass unaltered. One H atom is red to highlight the molecular orientation[2].

3. Dissolution of nanocrystals in solvents

167 ps methanol

Starting nanocrystal → Final liquid droplet
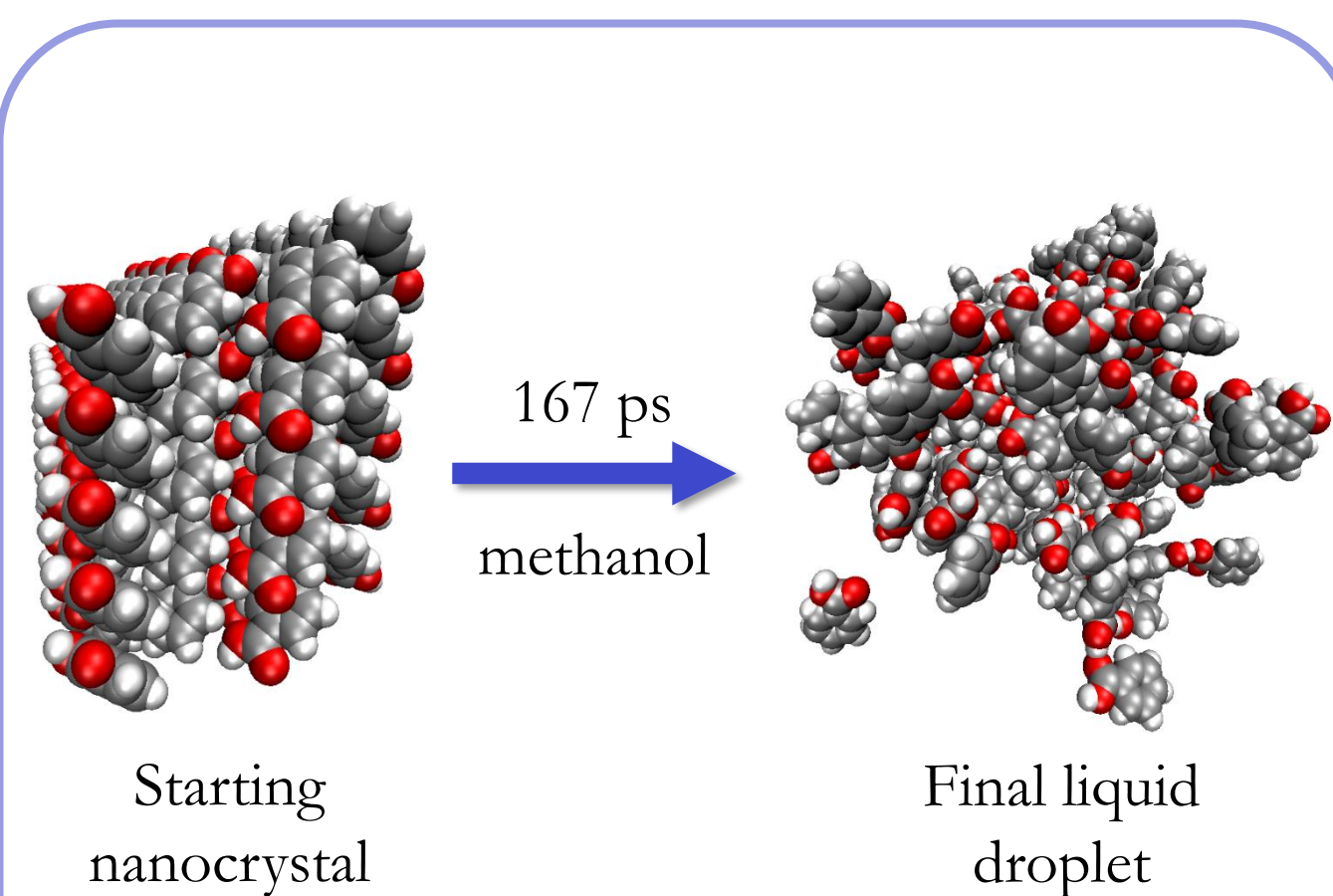
A benzoic acid nanocrystal loses its symmetry when immersed into pure methanol (not represented for clarity), suggesting that isolated clusters cannot be crystalline, contrarily to what is stated by CNT[5].

4. High density liquid transition in confined simulations

LD state / HD state / Nanocavity
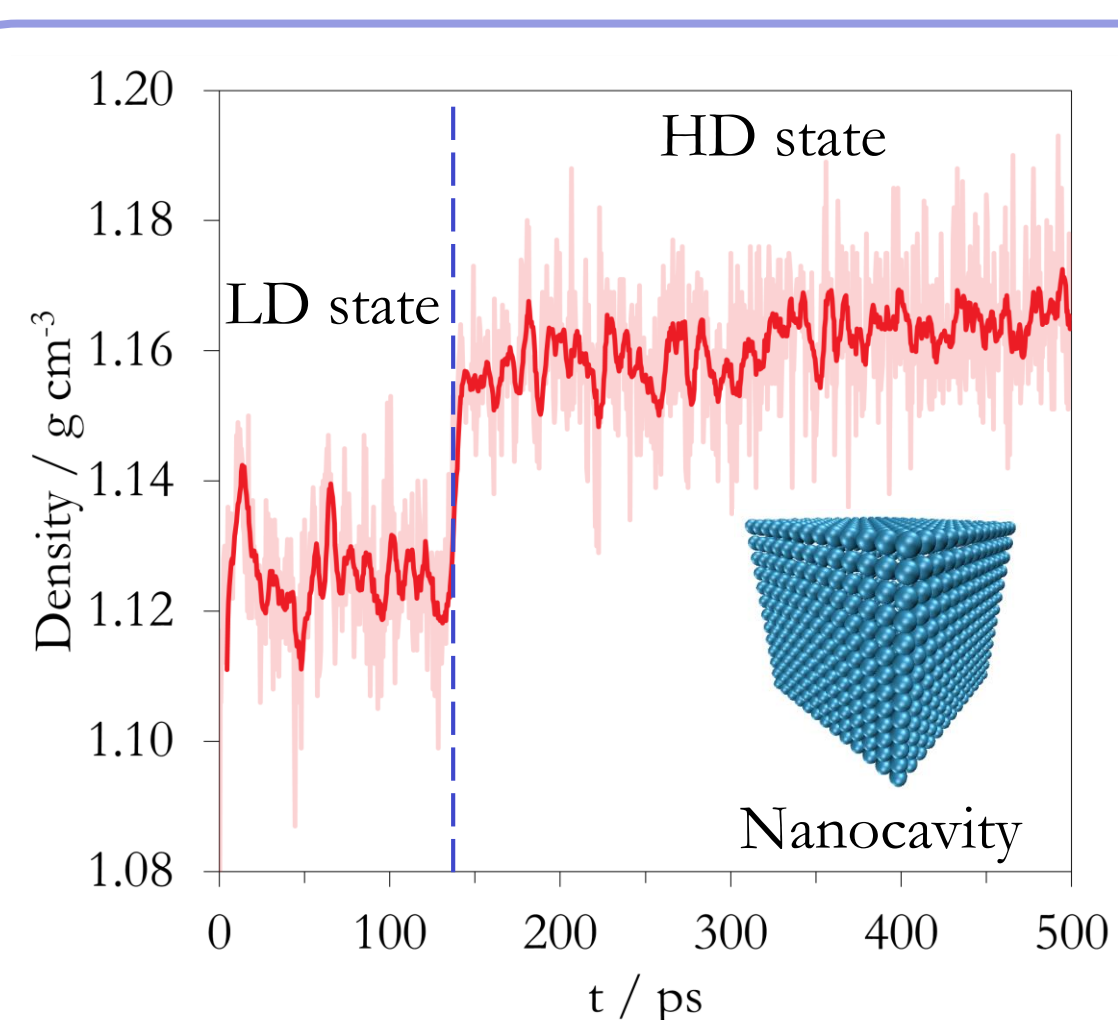
The confinement of liquid benzoic acid into a hydrophobic nanocavity with stiff barriers induces a reversible low density (LD) – high density (HD) transition towards a metastable state[6].

5. Time evolution of clusters in supercooled liquids
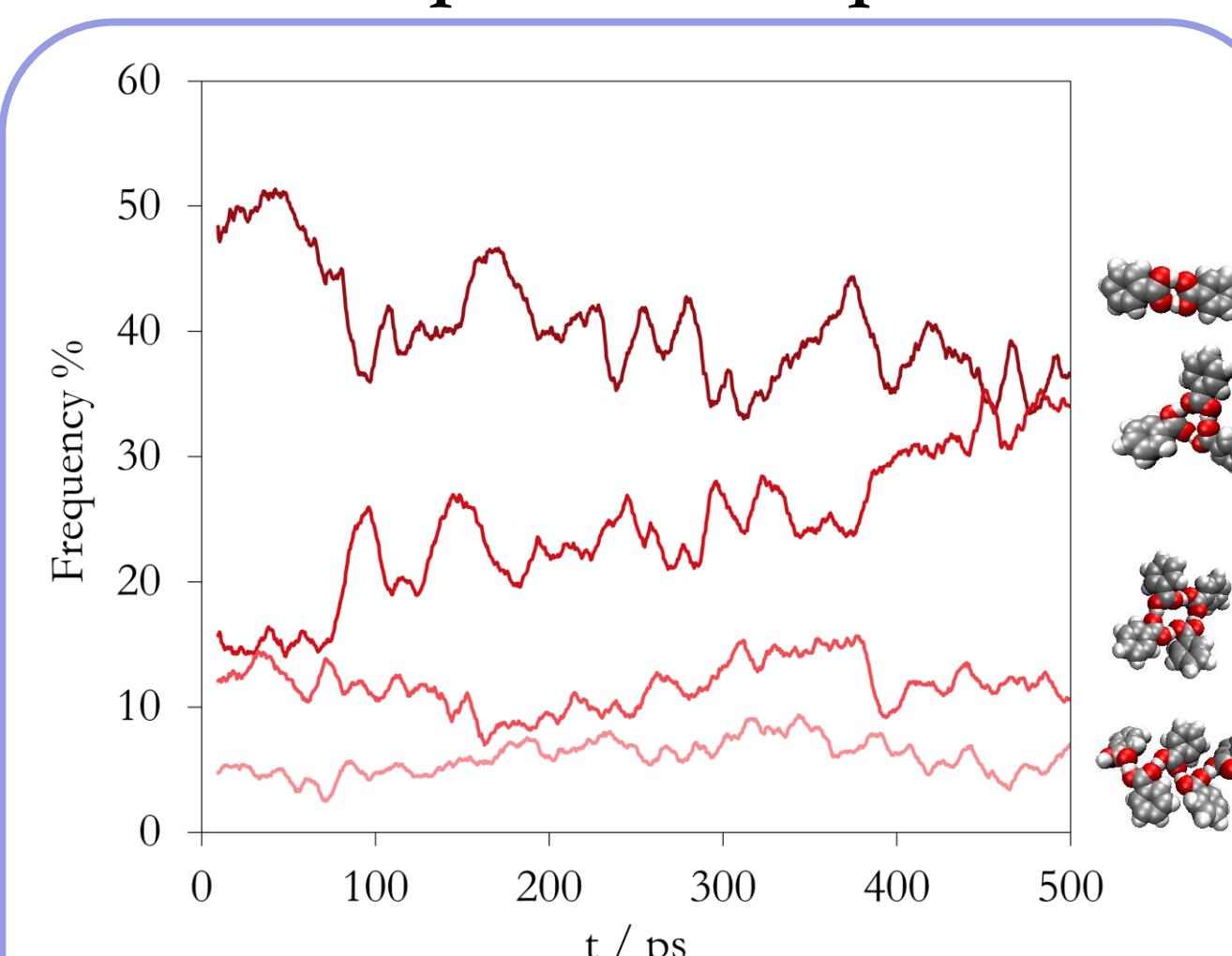
In supercooled benzoic acid, H-bonded dimers tend to decrease in favor of trimers. The amount of tetramers and pentamers, remains rather constant in time[7].

CONCLUSIONS

A quick assessment of some of MiCMoS functionalities has been conducted. MiCMoS represents a versatile tool to study molecular systems in the crystalline and liquid states, capable of addressing a wide range of challenges.
MiCMoS platform is continuously evolving and growing, and user input is deeply appreciated. Feedbacks are pivotal in fine-tuning the software to meet the specific needs of the users.

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12TH CRYSTAL FORMS @ Bologna — **September 10-12, 2023**

ACKNOLEDGEMENTS

ASSOCIAZIONE ITALIANA CRISTALLOGRAFIA