



September 28-29, 2026, Moscow

Computation of the Dielectric Properties of Molecular Systems in the **MULTICOMP** Package

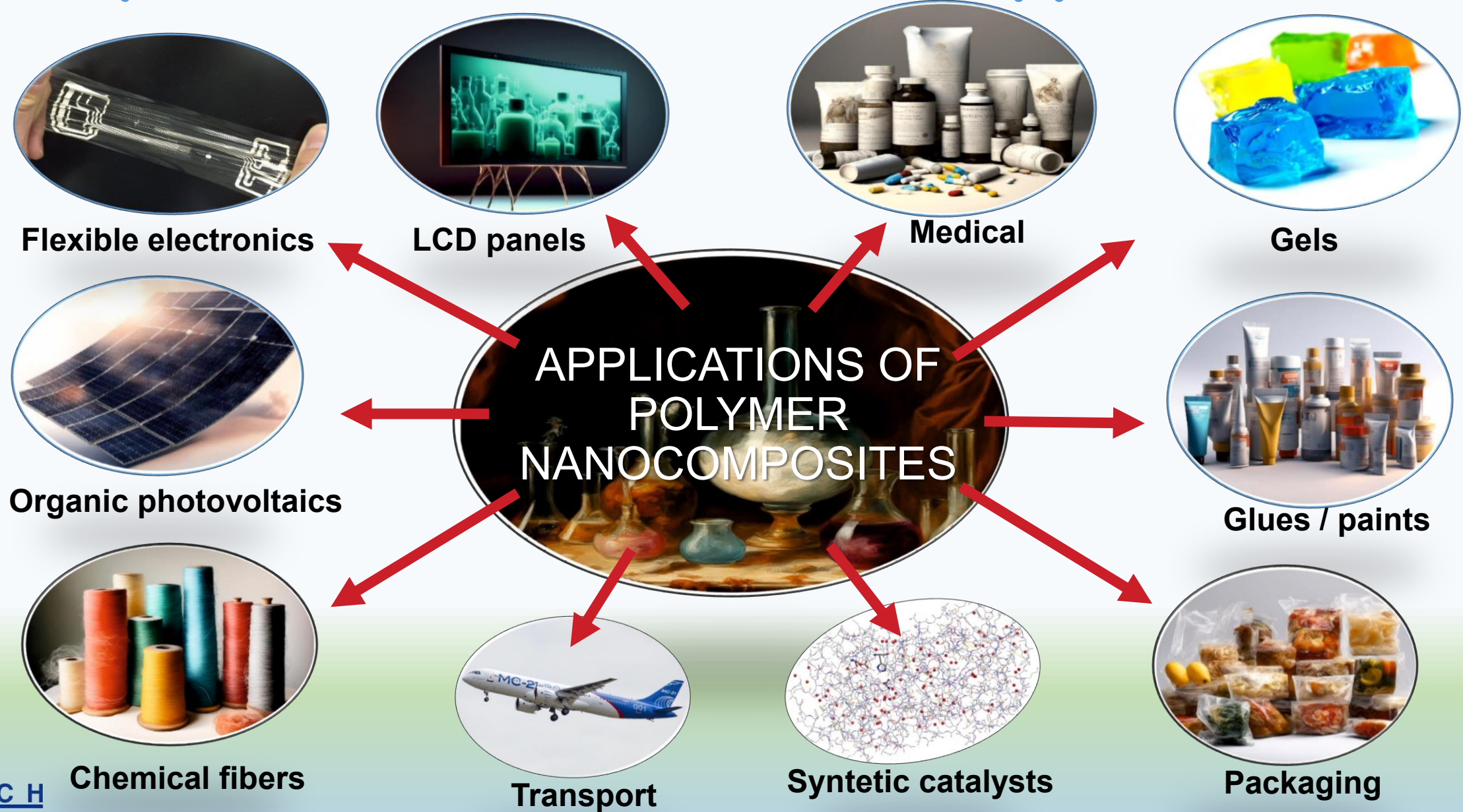
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Denis Shirabaykin¹, Sergey Trepalin¹ and Boris Potapkin¹

¹ Kintech Lab Ltd, Moscow, Russia; ²National Research Center "Kurchatov Institute", Moscow, Russia

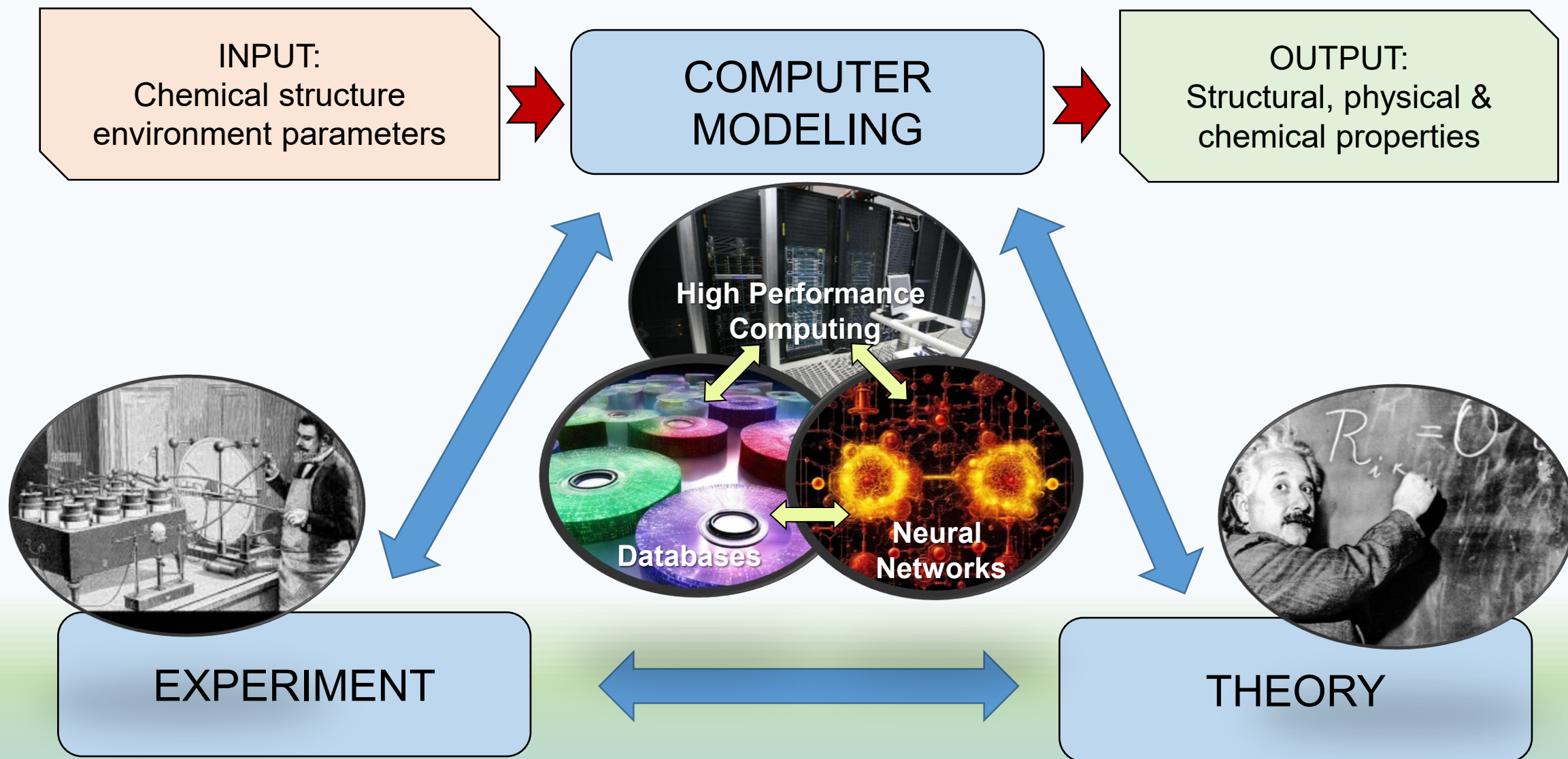
² Institute of Organoelement Compounds Moscow, Russia

The work is performed in Kintech Lab Ltd.

Polymer based materials: applications



Computer modeling in the development of new materials



Software for predictive modeling of polymeric material properties

GAMMESS



NWCHEM

HIGH-PERFORMANCE COMPUTATIONAL
CHEMISTRY SOFTWARE

LAMMPS

AMBER



GROMACS

FAST.
FLEXIBLE.
FREE.

Molecular Dynamics Simulations

HARMM

QUANTUMESPRESSO



MedeA

materials design

accelrys®

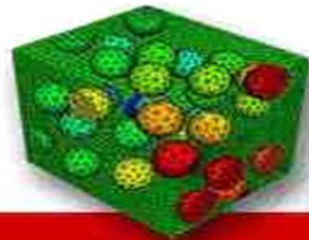


MATERIALS
STUDIO

Ultrasim®

BASF

OCTA



MSC Software

Digital

MesoProP

MULTICOMP software package for multiscale modeling of polymer-based materials

Designed for high-throughput materials screening on supercomputers



Working station



Supercomputer



input

- Chemical structure of components
- Geometry of nanoparticles and their properties
- Weight ratio of components
- Temperature, pressure and etc.



output

Physical properties of the material:

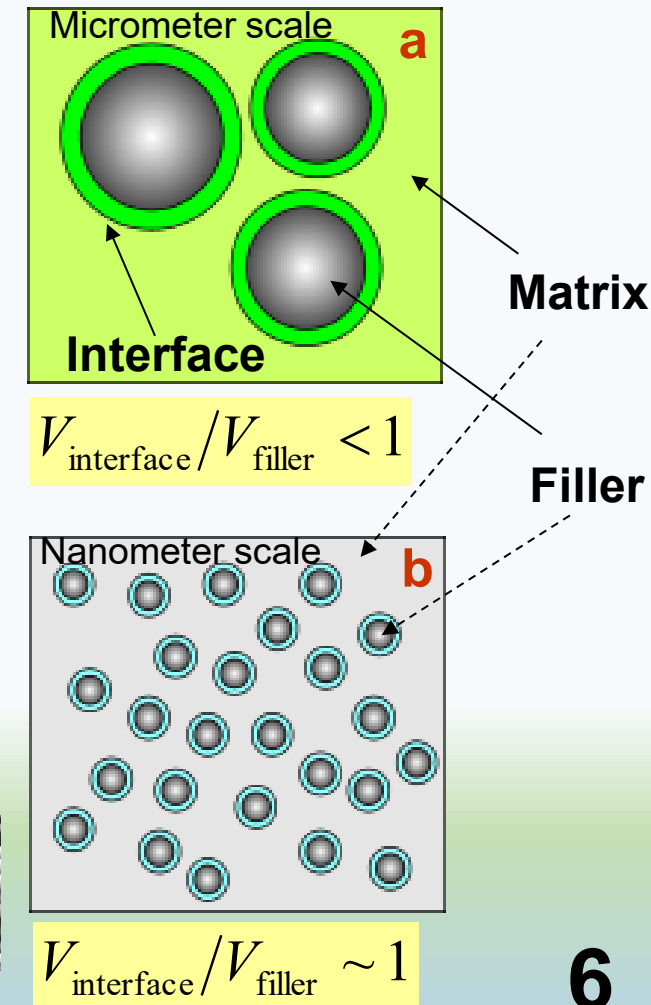
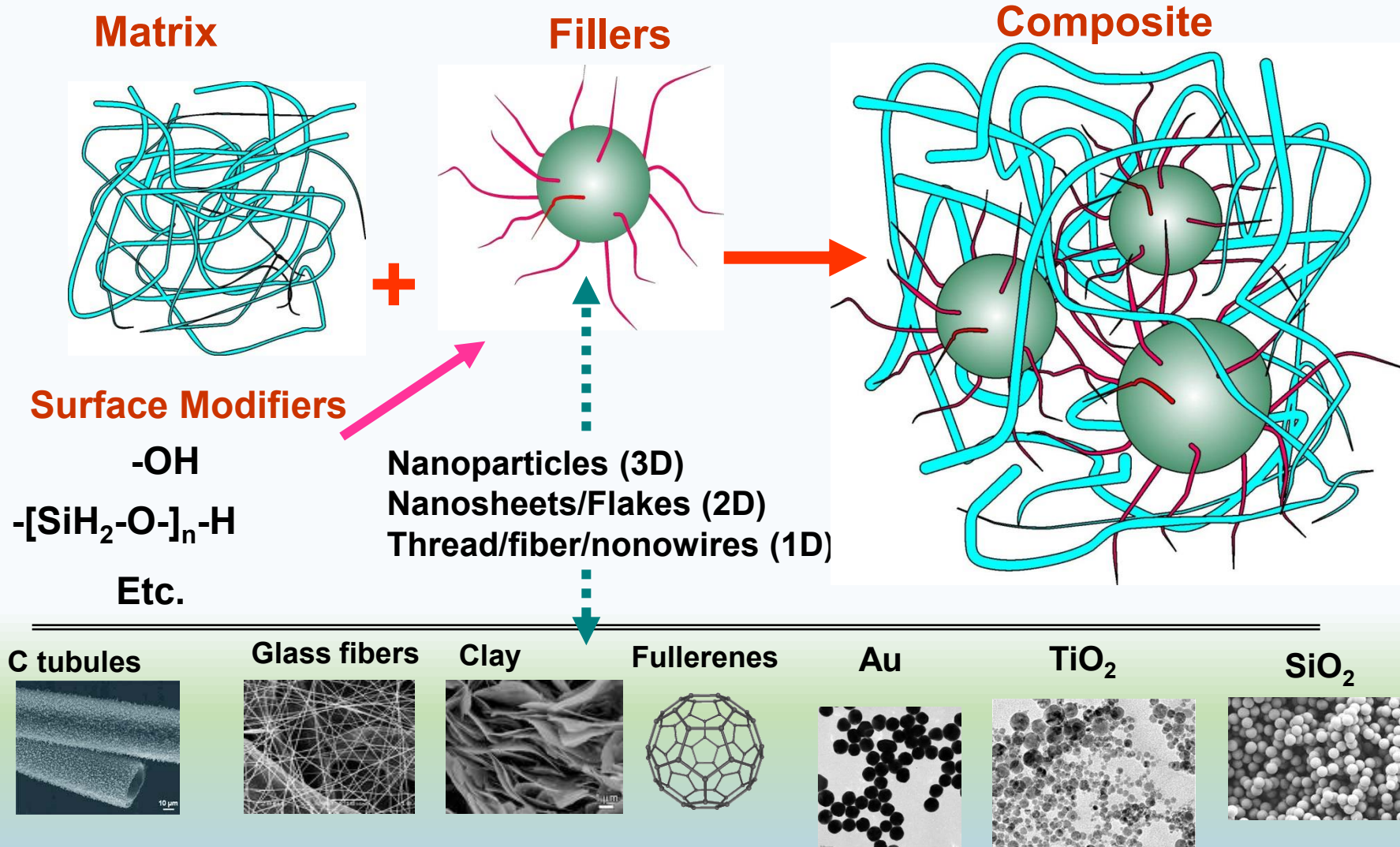
- structural
- mechanical
- thermophysical
- transport

M.A. Akhukov, V.A. Chorkov, A. A. Gavrilov, D.V. Guseva, P.G. Khalatur, A.R. Khokhlov, A.A. Kniznik, P.V. Komarov, M.V. Okun, B.V. Potapkin, V.Yu. Rudyak, D.B. Shirabaykin, A.S. Skomorokhov, S.V. Trepalin, **MULTICOMP** package for multilevel simulation of polymer nanocomposites, Computational Materials Science, V. 216, 2023, 111832, <https://doi.org/10.1016/j.commatsci.2022.111832>.

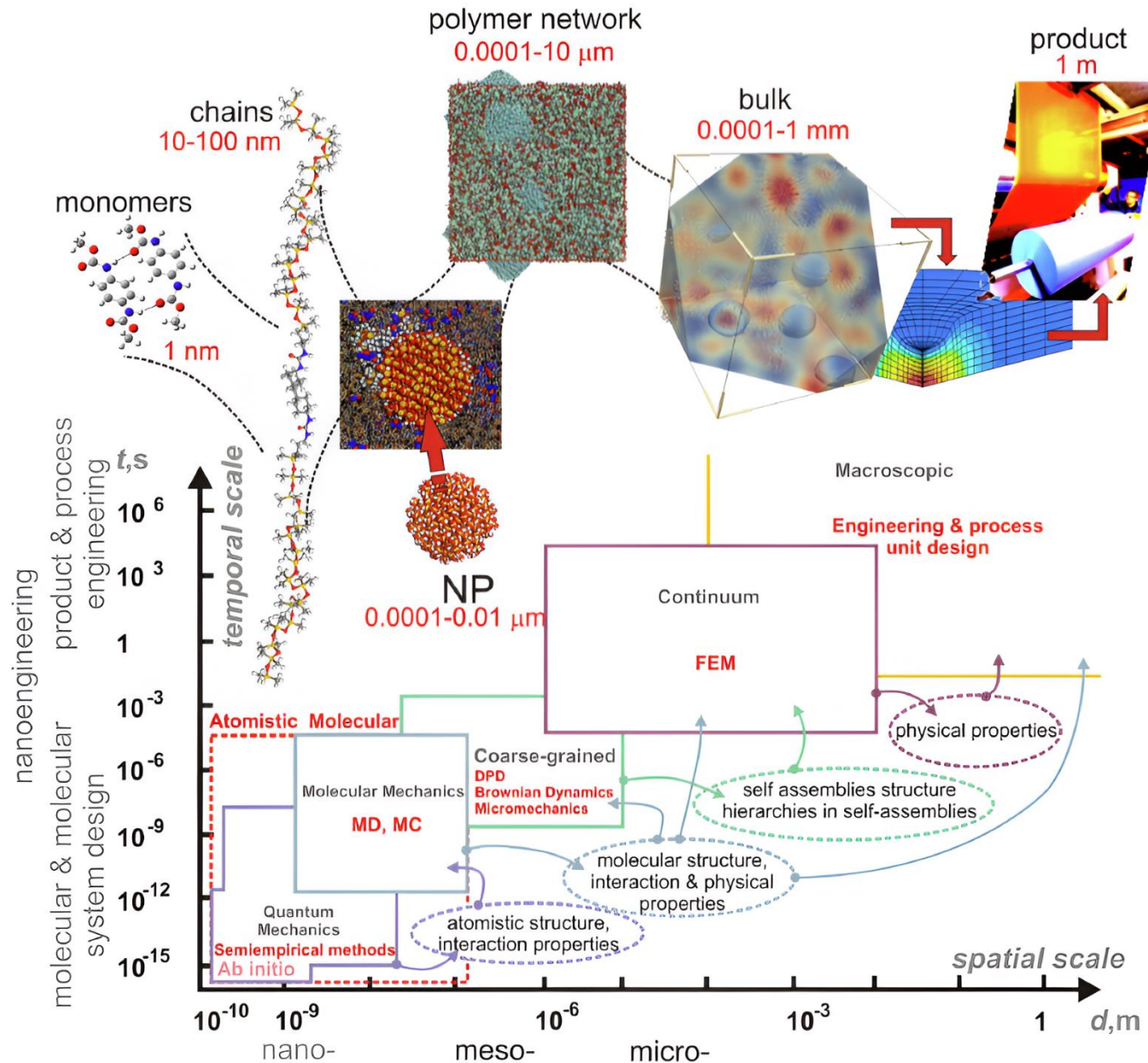
Polymer nanocomposites

Combination of a polymer matrix and filler that have at least one dimension (i.e. length, width, or thickness) in the nanometer size range ($1 \text{ nm} = 10^{-9} \text{ m}$)

- Composites** are materials consisting of two or more physically different phases, the combination of which leads to the emergence of new unique properties that differ from the characteristics of the original components.



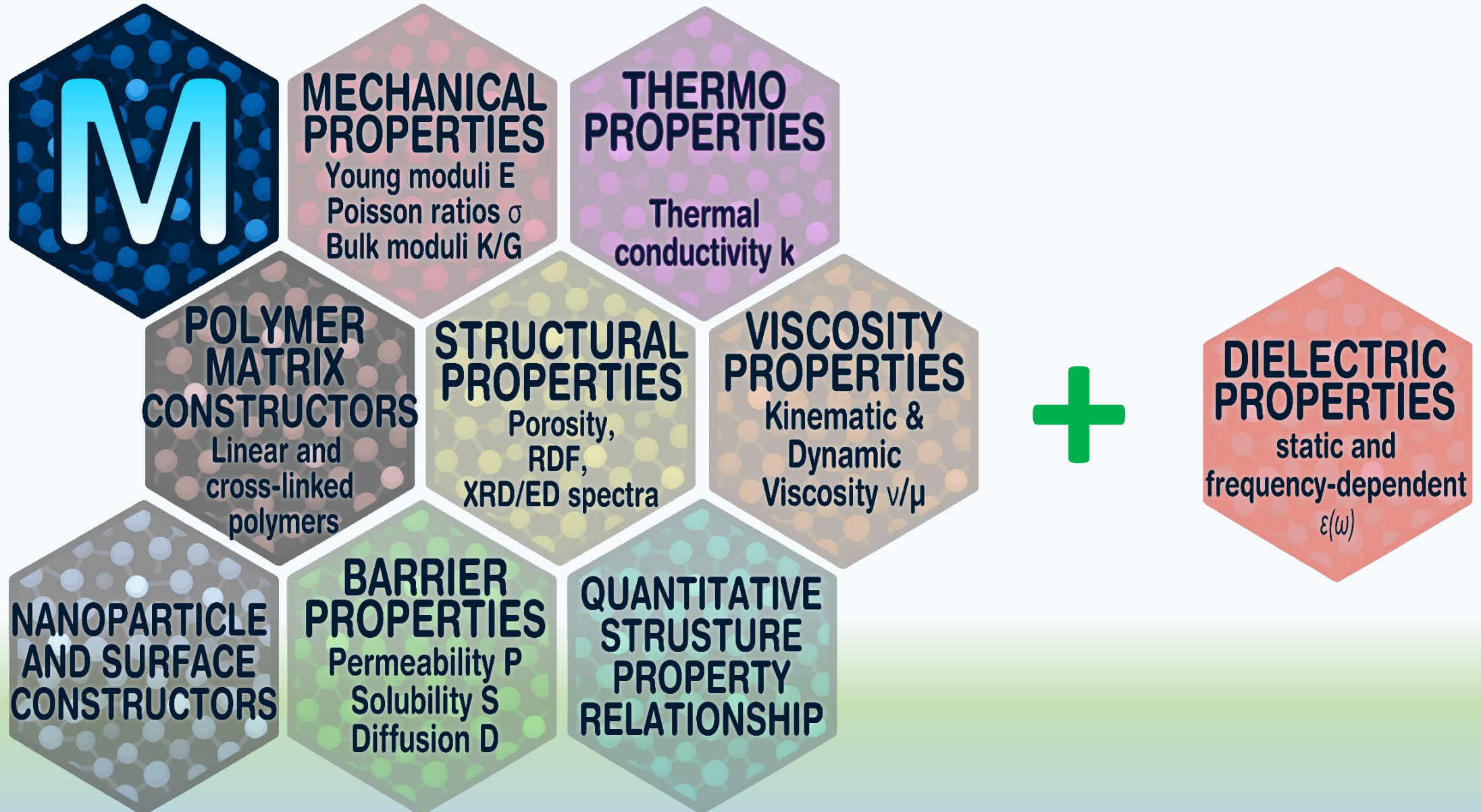
Polymer nanocomposites modeling: multiscale approach



In the case of nanocomposites, it is impossible within the framework of a one-level approach to combine high accuracy and large scale of consideration.

- **Atomistic level** - properties of nanosized filler and phase interaction
- **Mesoscale** - the distribution of the filler in the matrix
- **Macro level** - effective material properties

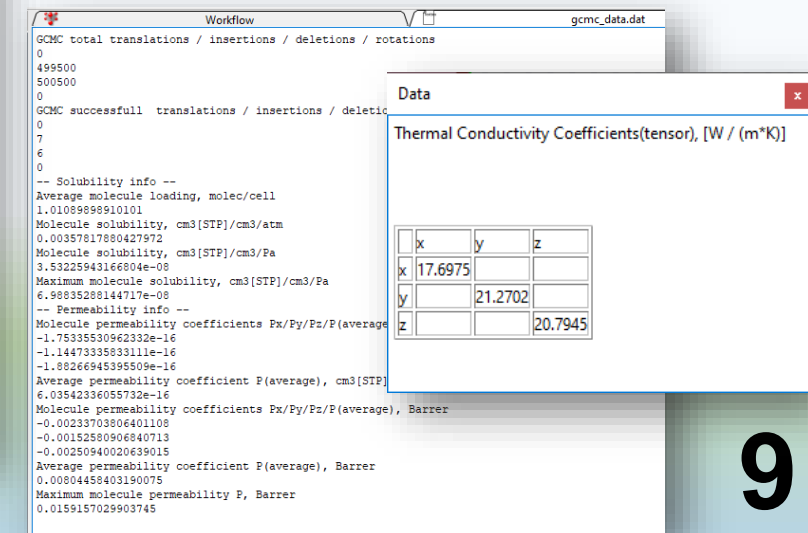
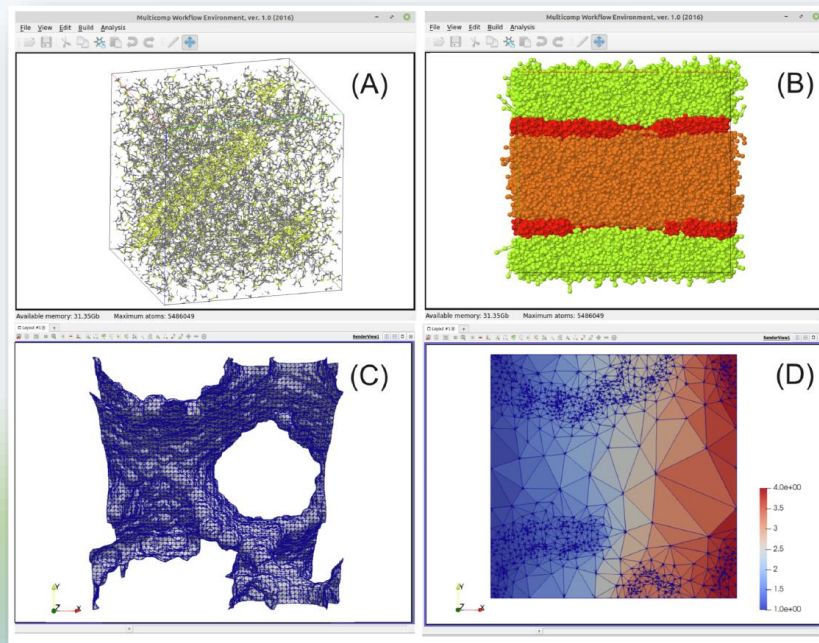
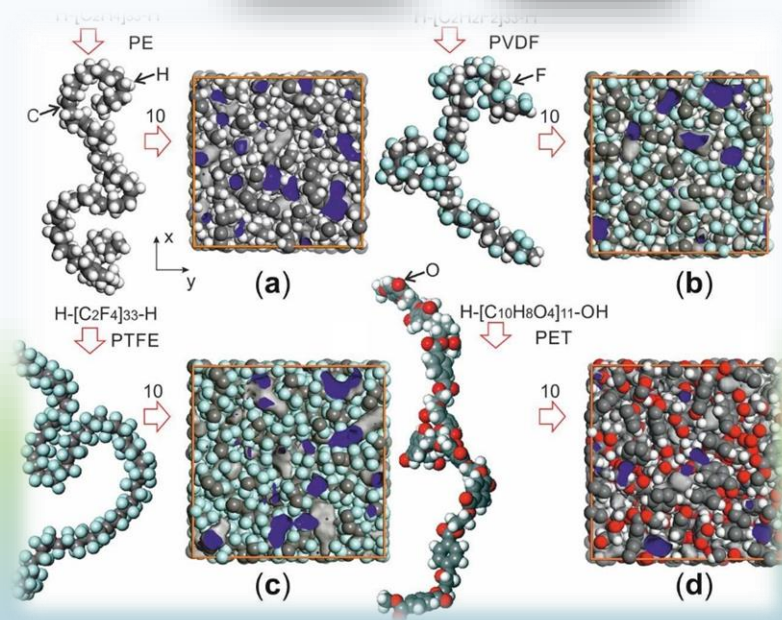
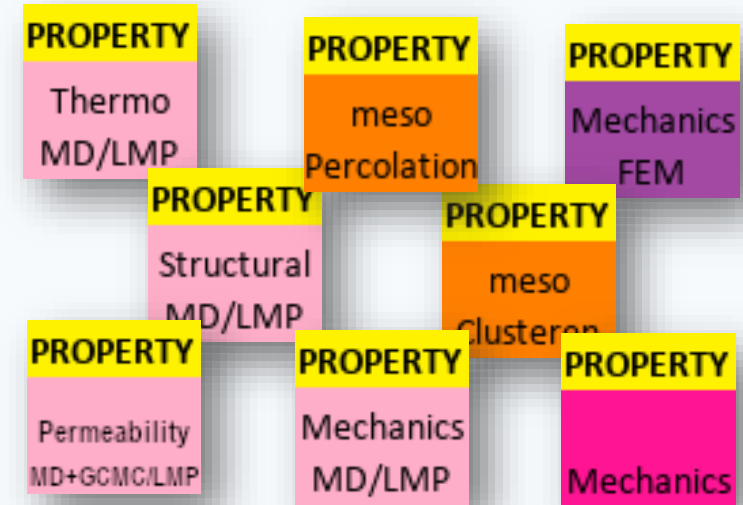
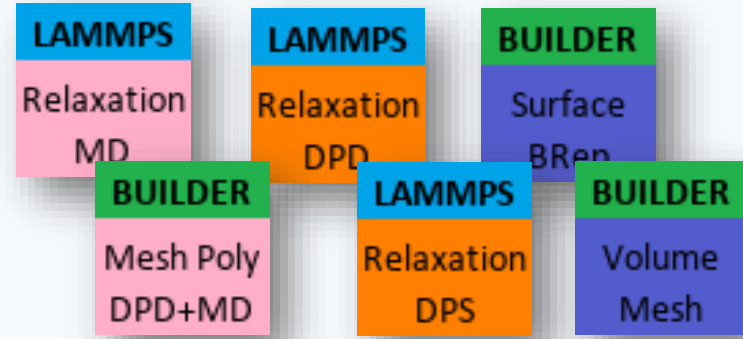
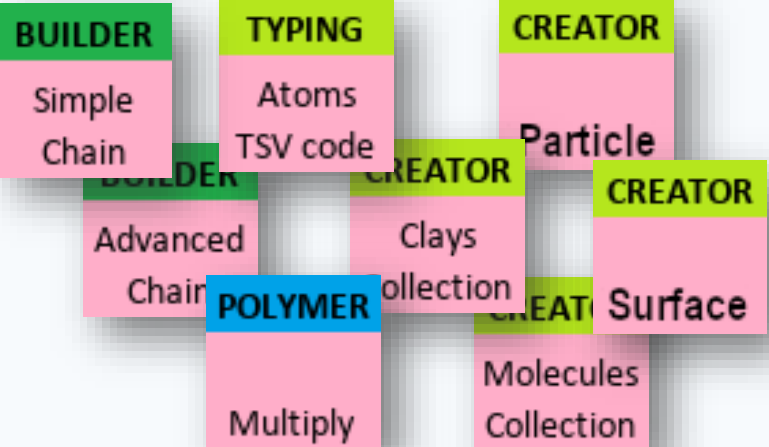
Multicomp Package Functionality



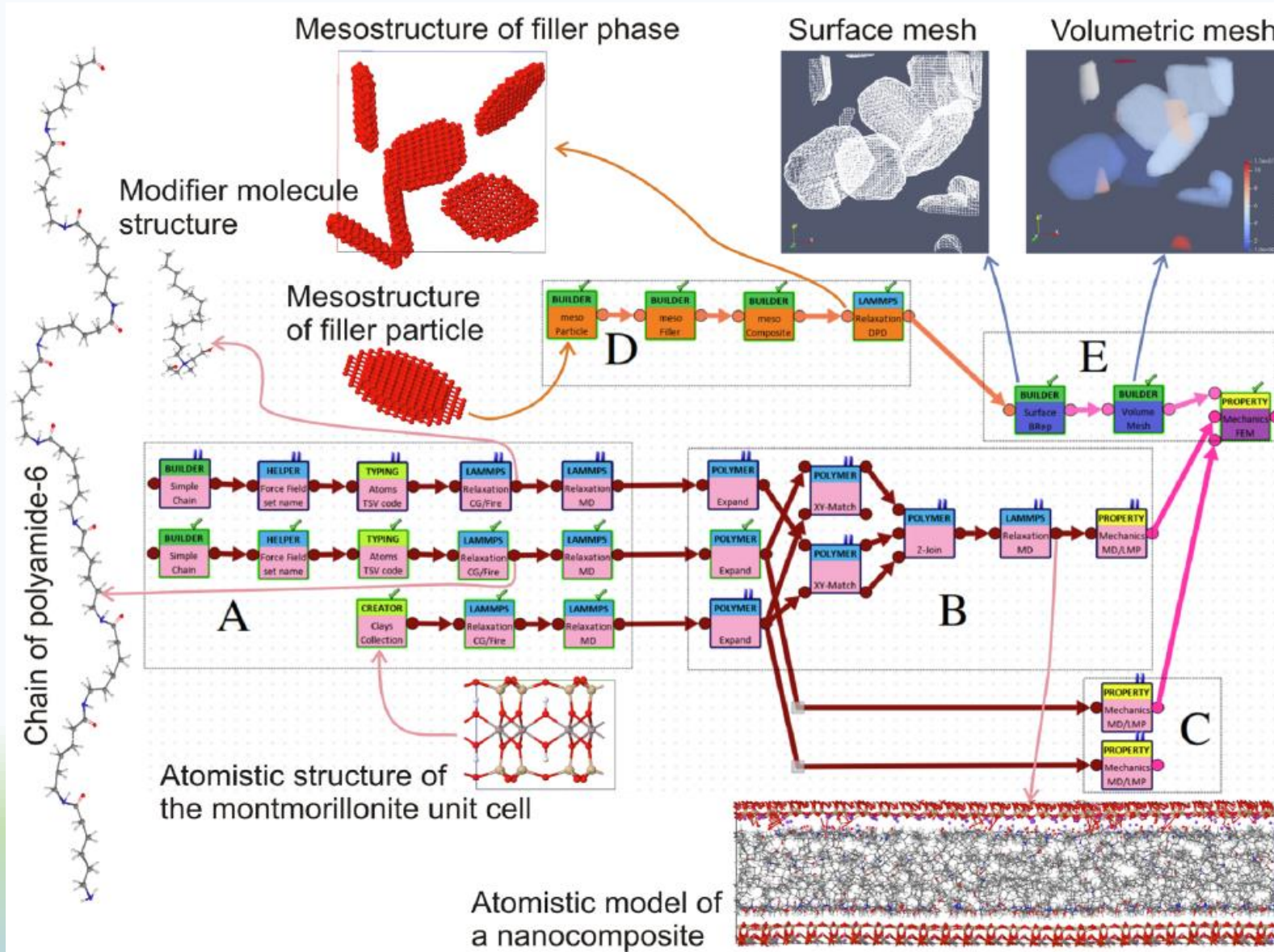
CHEMICAL COMPOSITION

MATERIAL MODEL

PHYSICAL PROPERTIES



Case study: multiscale calculation of macroscopic elastic modulus of the PA6-MMT nanocomposite



- ❖ The mechanical properties of the composite are different from the composition of the properties of the components due to the formation of a transition layer, whose elastic modulus is twice the elastic modulus of the matrix
- ❖ The increase in the elastic modulus of the material was 18% when filled by 1 wt.%. With the best structural parameters (experiment*), it is possible to increase the elastic modulus by up to two times
- ❖ The method is universal and allows you to calculate the properties of different structures: for an isotropic distribution of filler (1 and 100) module 4.2. and 11 GPa

Case study: gas barrier properties of multilayer polymer-clay nanocomposite films

STRUCTURE
DATABASE

QSPR PREDICTION

CANDIDATE SELECTION
PE / PET / PVDF / PTFE

SIMULATION
MD + GC MC

MACRO-LEVEL
MODEL

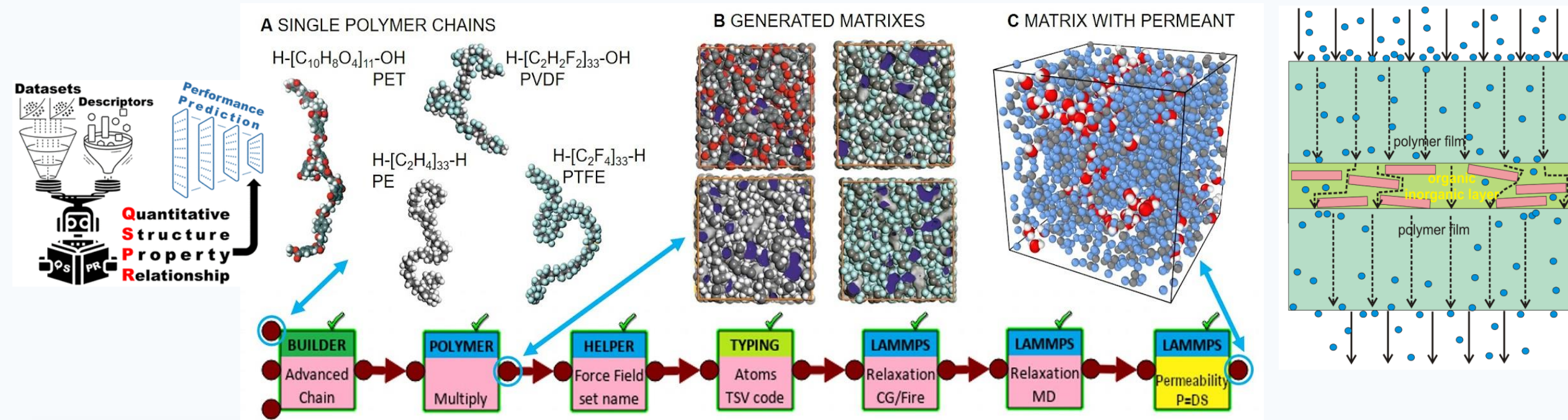
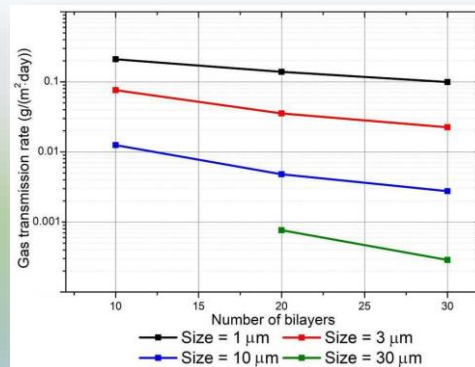


Table 4. Permeability coefficients of oxygen and water molecules for PET, PE, PVDF, and PTFE.

Material	$P(\text{O}_2)$ (Barrer)			$P(\text{H}_2\text{O})$ (Barrer)		
	MD-GCMC Simulations	Bicerano Model	Experiment [39,84]	MD-GCMC Simulations	Askadskii Model	Experiment [39,84]
PET	0.01–0.02	0.04	0.013–5	1–2	87	100–1300
PE	0.2–0.6	4.47	0.04–5	2–12	60	20–75
PVDF	0.07–0.2	8.91	0.02–1.8	8–30	193	–
PTFE	17–22	7.65	2.5–6	10–50	328	3–8



✓ Successful candidate selection
before synthesis

✓ Determination of the optimal filler
aspect ratio using macro-level model

Where dielectric properties calculation usually lives

- **DFT packages:** VASP, Quantum Espresso, via linear response / post-processing
- **MD-trajectory tools:** MAICoS, MDTraj, GROMACS built-in utility
- **Limitation:** each addresses only an isolated stage

What's new in **MULTICOMP**

- Integrated into the multiscale modeling of polymeric materials
- **Extensive built-in postprocessing** using several approximations
- **Effective HPC usage:** time-intensive runs sent to remote clusters through the interface

What the module implements

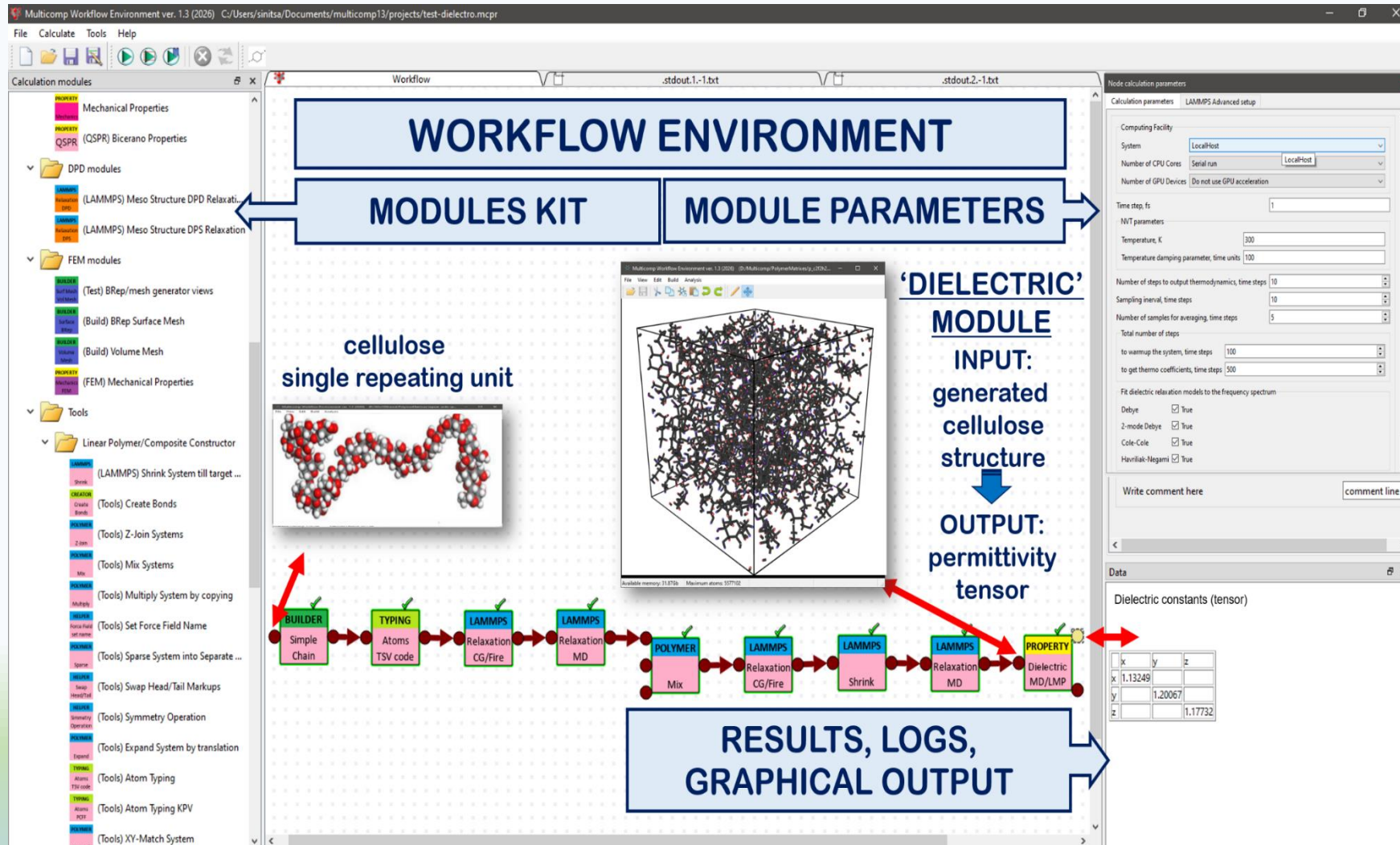
- **Static ϵ_0 :** Kirkwood fluctuation formula [1-3]
- **Complex $\epsilon(\omega)$ spectrum:** Neumann velocity–dipole formalism [4]
- **Relaxation fitting:** single & two-mode Debye, Cole–Cole [5], Havriliak–Negami [6-8] (with introduced physical constraints)
- **Dielectric loss:** analytical calculation for loss tangent $\tan(\delta)$

PROPERTY

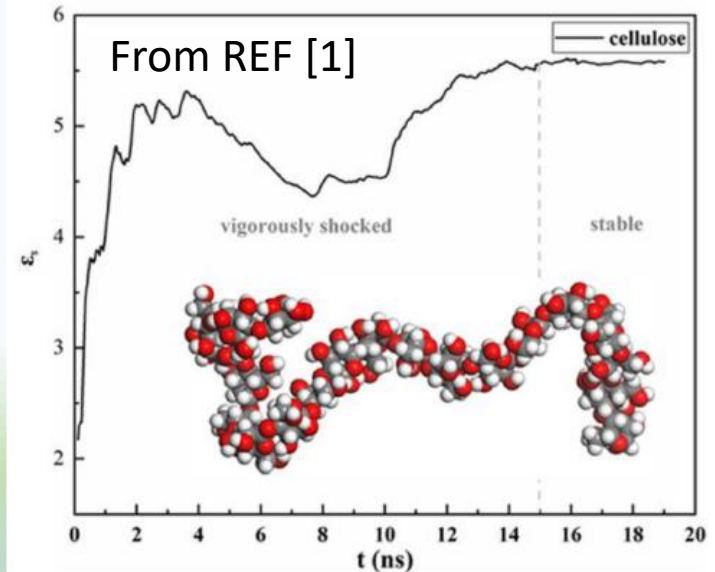
Dielectric
MD/LMP

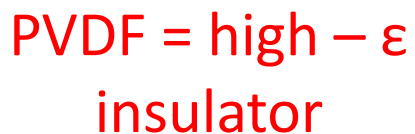
Module verification: dielectric permittivity of cellulose

Cellulose as the test system: one of the most extensively studied biopolymers and critical in electrical insulation applications (oil-paper insulation systems in transformers)



✓ MD simulations with **COMPASS FF**
✓ Good agreement with [1]:
 $\epsilon(0) = 6.3 \pm 0.66$ for the cellulose type U

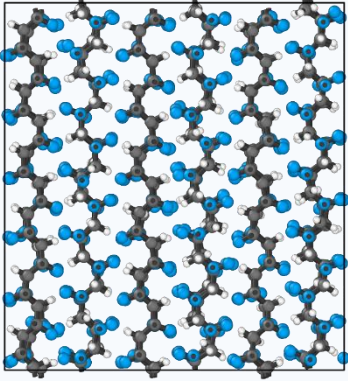




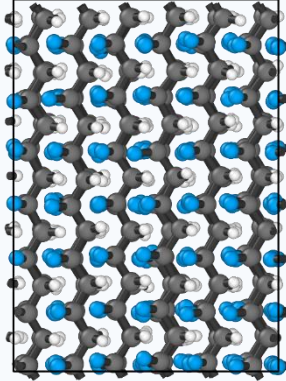
PVDF is a high-performance insulating polymer whose dielectric constant and energy losses vary significantly depending on its crystal phase (α , β , δ or γ) and the applied electric field frequency.

Case study: calculating the Dielectric Properties of Polyvinylidene fluoride (PVDF)

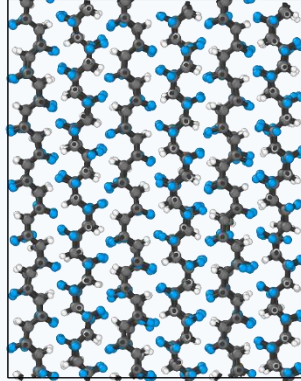
crystal α -phase



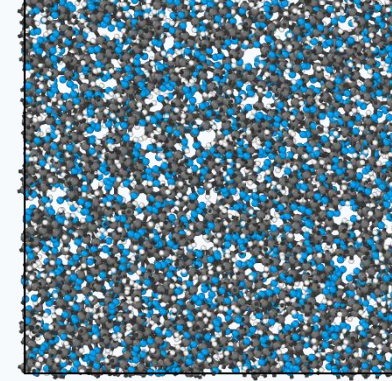
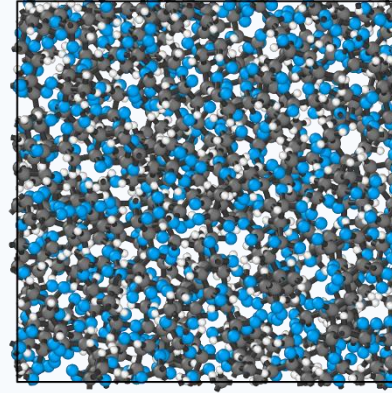
β -phase



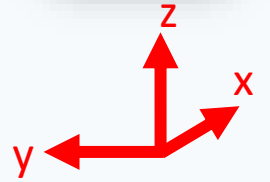
δ -phase



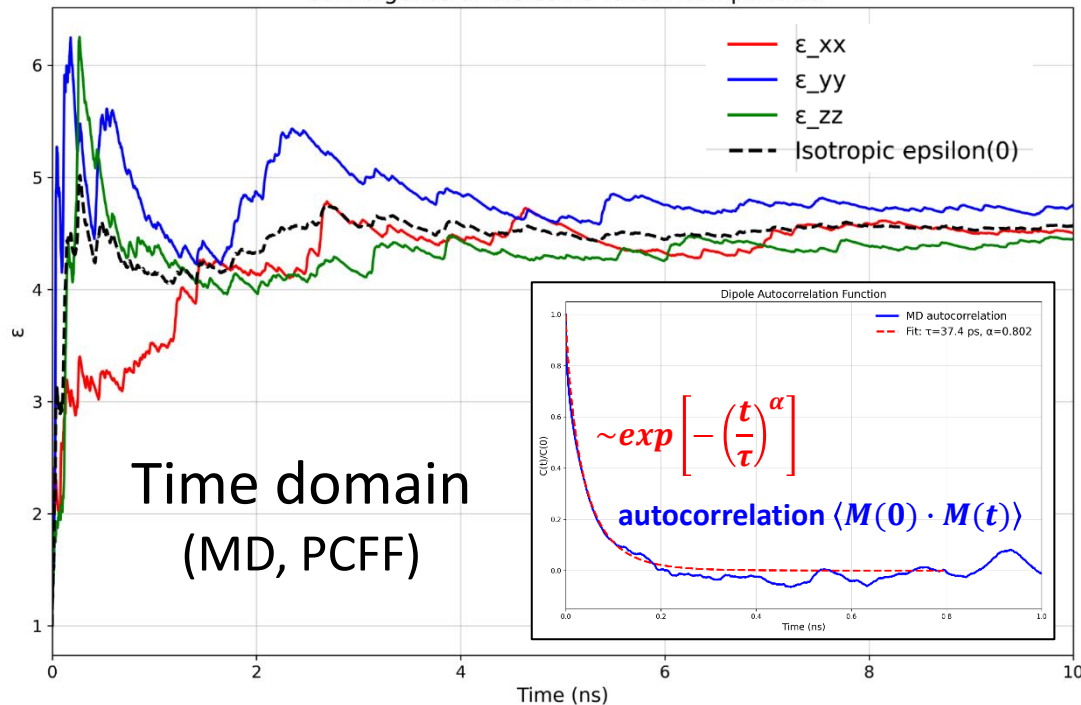
amorphous PVDF



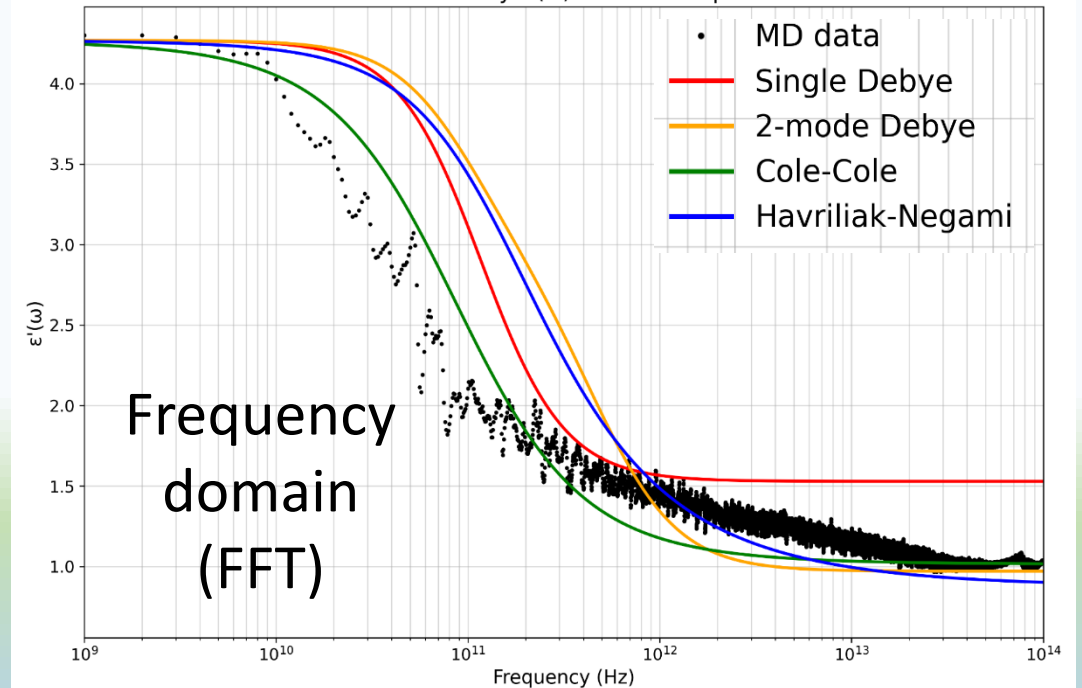
PROPERTY
Dielectric
MD/LMP



Convergence of Dielectric Tensor Components



Real Permittivity $\epsilon'(\omega)$ - Model Comparison



Calculated PVDF dielectric properties

System	PVDF α -phase	PVDF β -phase	PVDF δ -phase	PVDF amorphous (2000 atoms)	PVDF amorphous (5460 atoms)
ϵ_{xx}	1.28	1.27	1.24	2.83 $\pm$ 0.27	4.40 $\pm$ 0.32
ϵ_{yy}	1.20	1.05	1.15	3.42 $\pm$ 0.33	4.65 $\pm$ 0.38
ϵ_{zz}	1.18	1.10	1.17	3.03 $\pm$ 0.29	4.34 $\pm$ 0.33
Isotropic ϵ_0	1.22	1.14	1.19	3.1 $\pm$ 0.25	4.46 $\pm$ 0.33
Debye model tan(δ)	0.46	0.42	0.44	0.43	0.53
$f_{\max}$ (KWW eq.)	2.65 GHz	2.49 GHz	2.6 GHz	3.9 GHz	3.85 GHz

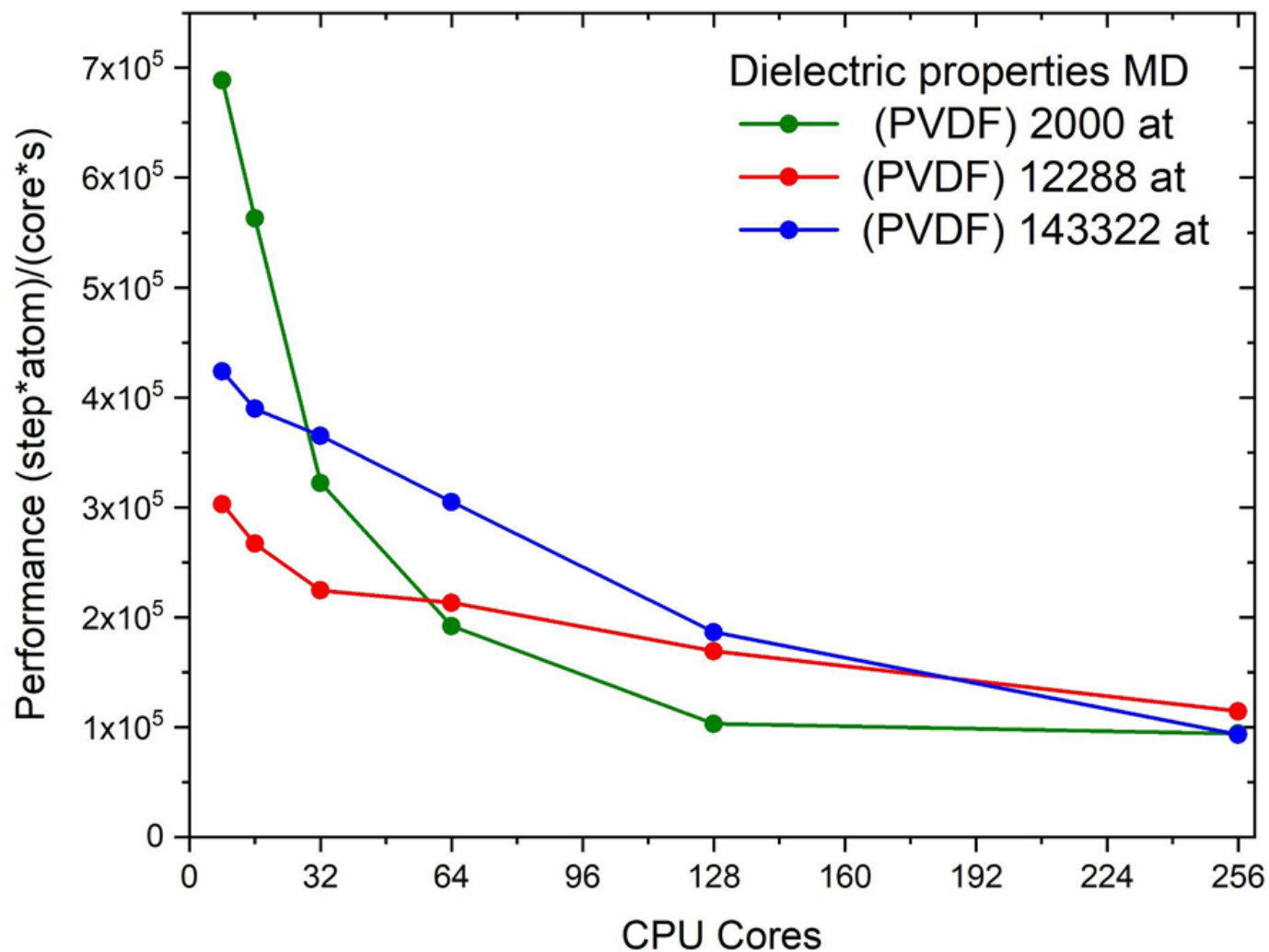
•**Crystalline phases:** low and similar dielectric permittivity.

•**Amorphous PVDF:** significantly higher permittivity, with $\epsilon_{\text{amorphous}} / \epsilon_{\text{crystal}} \approx 4$ [Macromolecules, Vol. 28, No. 20, 1995].

•**System-size effect:** larger amorphous models better capture dipolar correlations and conformational disorder.

✓ The simulations reproduce the experimentally observed strong dependence of PVDF dielectric properties on molecular morphology.

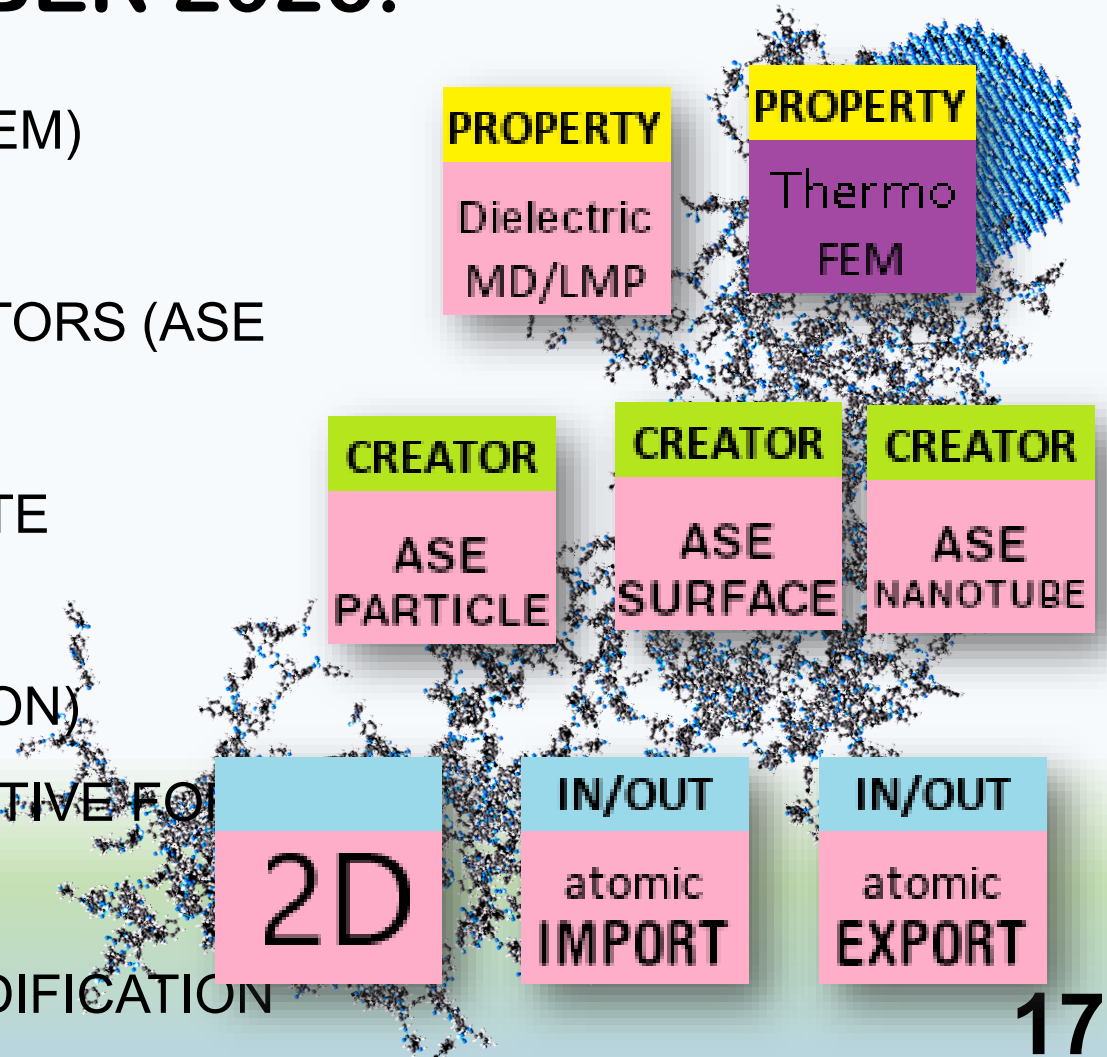
- **Long MD trajectories:** Reliable low-frequency dielectric properties require **~10–100 ns simulations** to converge dipole fluctuations and autocorrelation functions.
- **CPU scalability:** $\sim 7 \times 10^5$ atom-steps/(core·s) for a 2,000-atom PVDF system; $\sim 3\text{--}4 \times 10^5$ atom-steps/(core·s) maintained for systems up to 143,328 atoms.
- **GPU acceleration:** $\sim 2 \times 10^5$ atom-steps/(core·s) achieved on NVIDIA RTX 3090 GPUs, enabling efficient large-scale dielectric simulations.



Conclusion remarks

- **A new Dielectric Properties module** has been developed and integrated into the MULTICOMP software package, enabling equilibrium-MD calculations of static and frequency-dependent dielectric permittivity, dielectric loss, and characteristic relaxation times.
- The module within MULTICOMP provides an **integrated end-to-end workflow**, from automated construction of realistic polymer and nanocomposite models to dielectric-property prediction, improving the efficiency and reproducibility of multiscale simulations.
- **Validation on cellulose and PVDF** demonstrates the reliability of the implemented methodology, including good agreement with published static dielectric permittivity data for cellulose.
- **For PVDF**, the simulations reproduce the strong morphology dependence of dielectric response, most notably the substantially higher permittivity of amorphous phases compared with crystalline polymorphs. Frequency-dependent spectra and relaxation analysis provide additional insight into dipolar and segmental dynamics and demonstrate the capability of the module to characterize complex dielectric relaxation behavior.
- **Overall**, MULTICOMP provides a practical computational framework for virtual screening, design, and optimization of advanced dielectric polymer and nanocomposite materials.

- INTRODUCING DIELECTRIC (MD) AND THERMO (FEM) PROPERTIES MODULES
- EXTENDED SURFACE AND PARTICLE CONSTRUCTORS (ASE LIBRARY)
- MODIFIED VERSION OF THE DPD NANOCOMPOSITE CONSTRUCTOR MODULE
- UPDATED LAMMPS MD ENGINE (JULY 2025 VERSION)
- ADDED SUPPORT FOR USER-DEFINED AND REACTIVE FORCE FIELDS (ReaxFF)
- IMPROVED VISUALISATION AND STRUCTURE MODIFICATION TOOLS



Thank you for your attention!



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acknowledgments

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