

Journées Annuelles PEPR LUMA



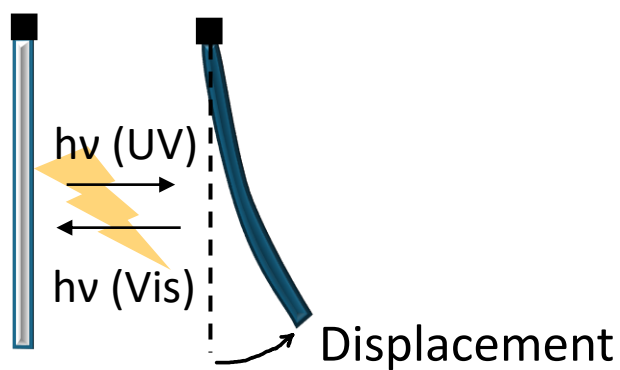
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SIMULACTOR

Multi-Scale Simulations of Polymeric PhotoActuators

Polymeric photoactuators (PPA)
= thermoplastic elastomer + organic
photochromes



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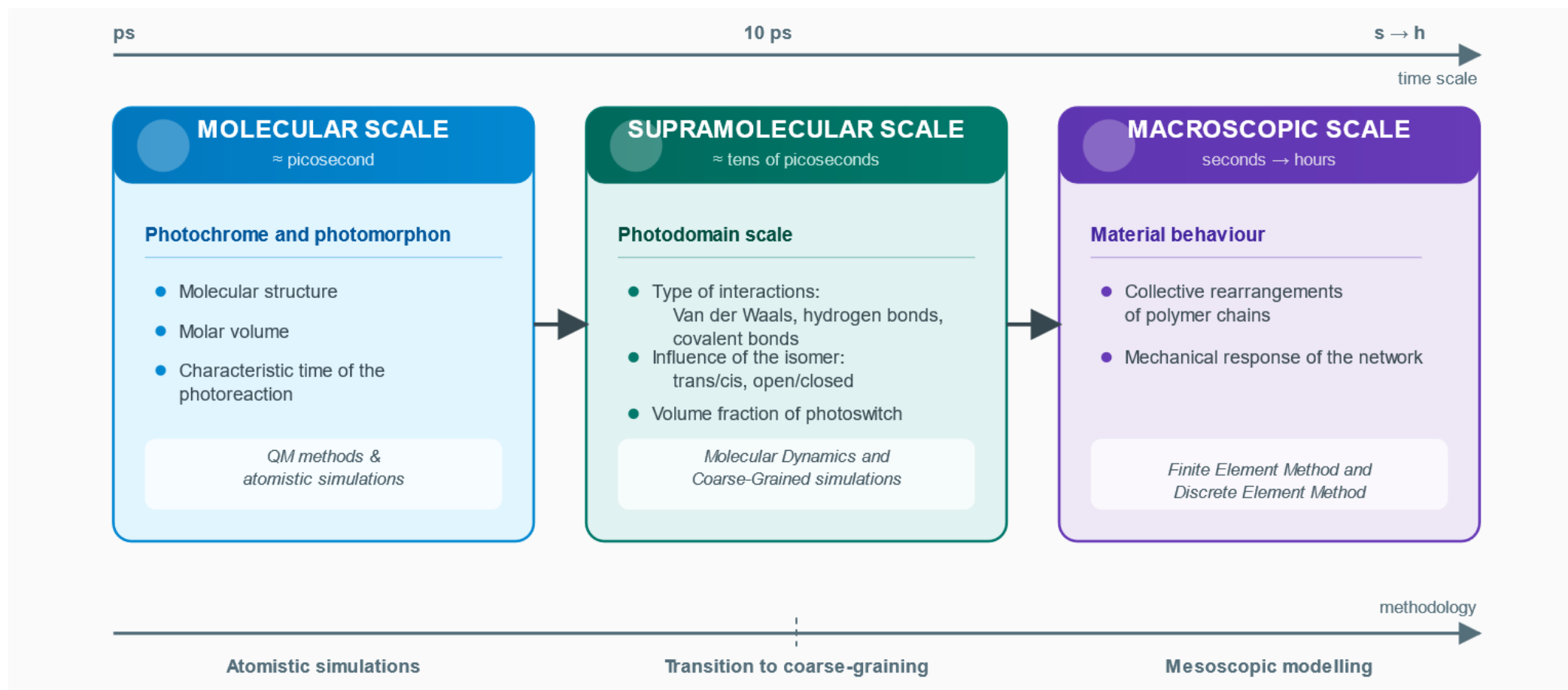
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- Behavior of these materials at the **molecular, supramolecular and macroscopic scales?**
- **Integrated multi-scale approach** to model the mechanical behavior of PPAs

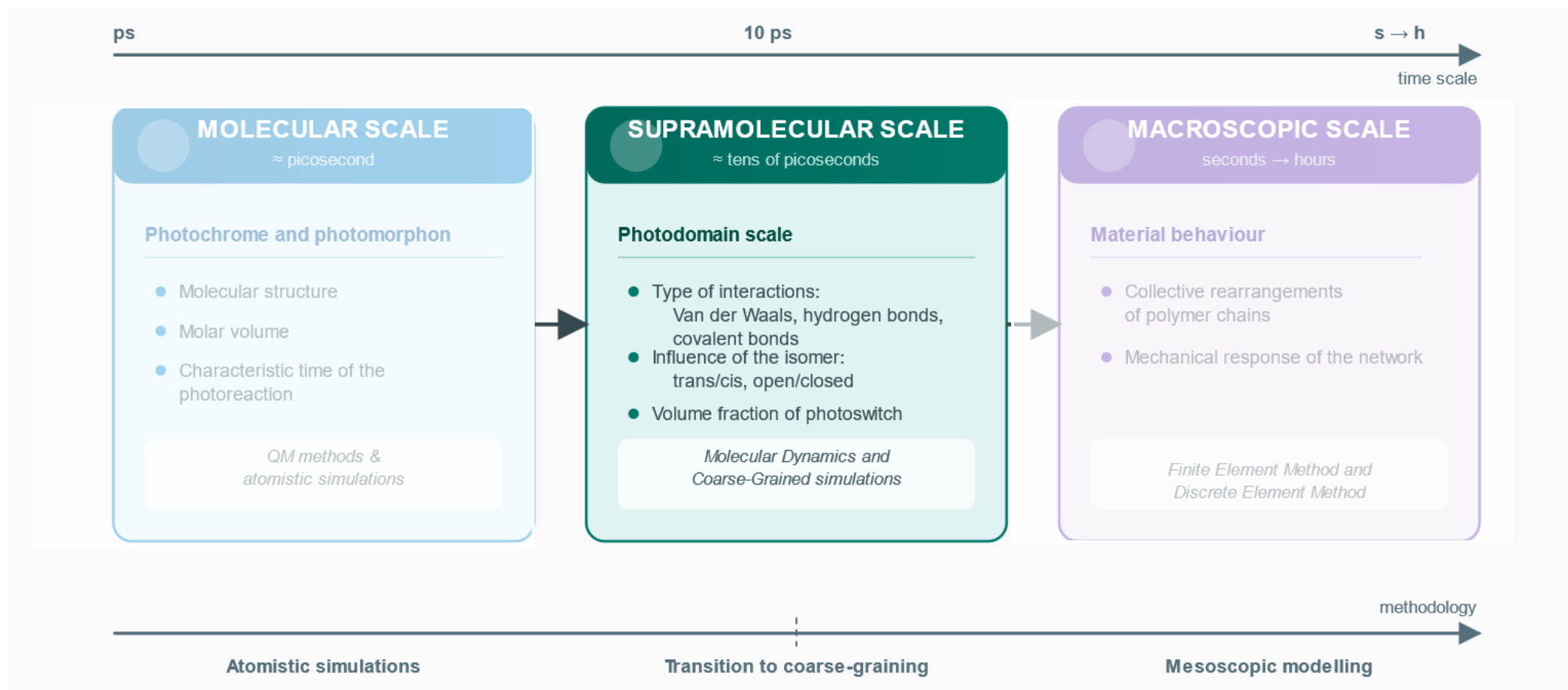
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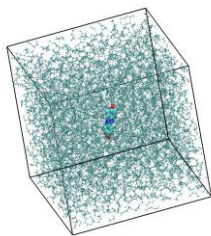
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Does the photoreaction
change the micro-
properties of the matrix?



Local pressure $\langle P \rangle$

Atomic displacements Δr

Angular displacements $\Delta \chi$



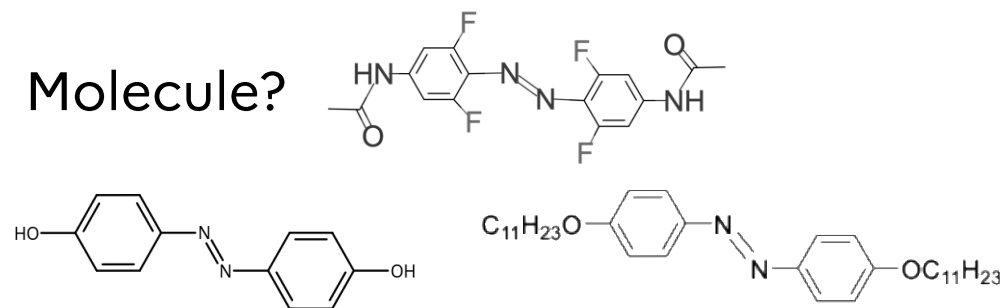
Does the matrix impact the
photoreaction?



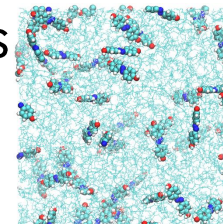
M. Serrano Martínez, N. Pineau, C. A. Lemarchand, A. Perrier;
Phys. Chem. Chem. Phys. **2025**; 27 (44): 23669–23684

- Strategy? Reaction coordinate?

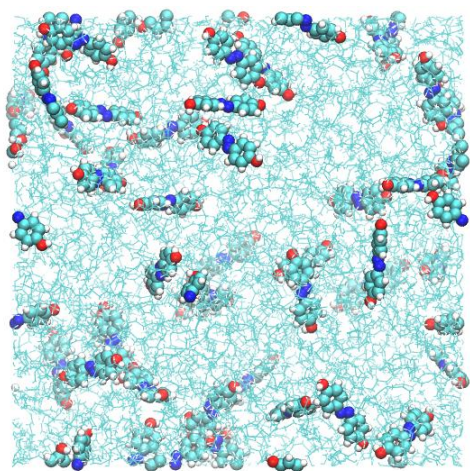
- Molecule?



- Number of molecules
20, 50, 200 photochromes



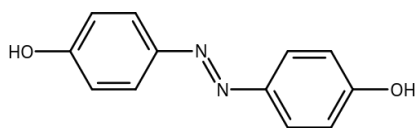
Variation of the volume / box size as a function
of the photochrome concentration ?



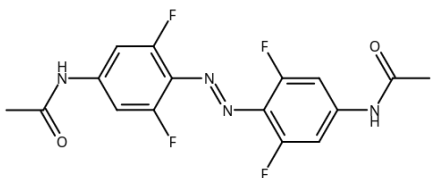
72 polymer chains - Polybutadiene
Average 30 monomers/chain

NPT simulations

AZ-OH



F-Azo



Specific volume, bulk modulus & viscoelastic moduli

vs. *Concentration* (20, 50, 200 photochromes)
and *isomer* (cis / trans)

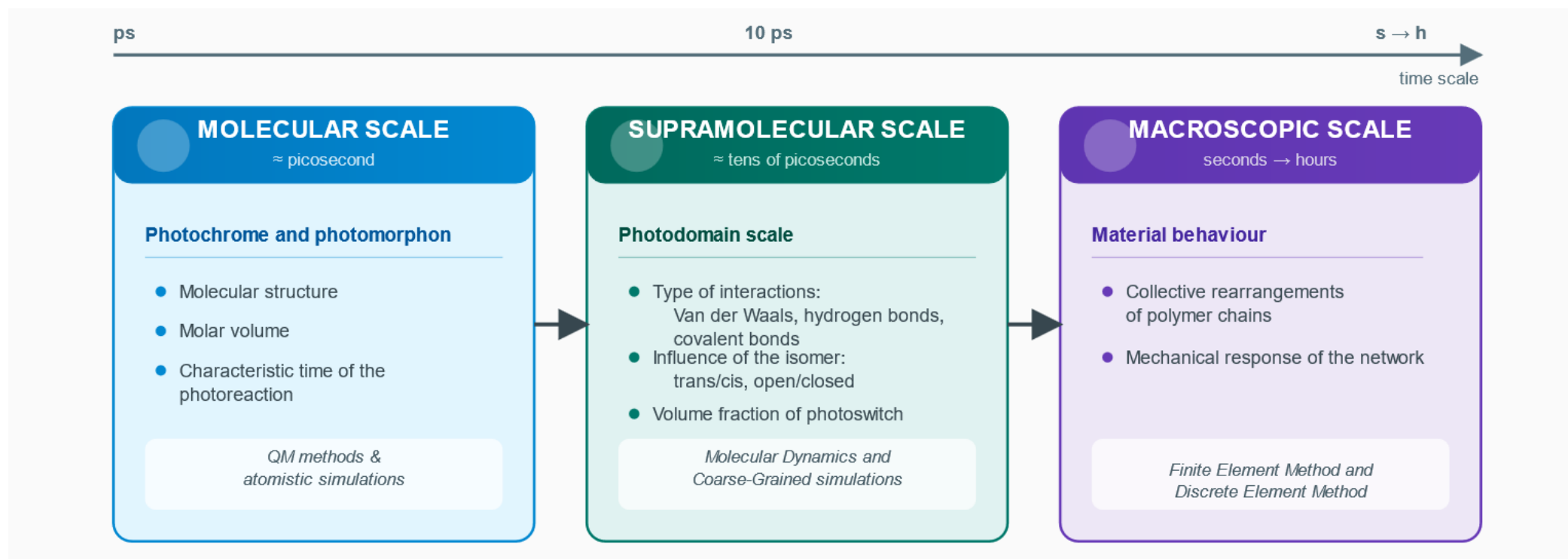
- **Bulk modulus:** high at all concentrations, consistent with experiments
- **Time-dependent viscoelastic moduli:** isomer- & concentration-dependent at short times (~ 1 fs); no dependence at long times (~ 1 ns)
- Surprising finding: **no cis/trans difference in specific volume**

➔ **New polymer? Dynamics of the phenomenon?**

M. Serrano Martinez, N. Pineau, A. Pierron de Mondésir, M. Nait-Abdelaziz, A. Perrier, C. A. Lemarchand, in revision

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Starting date 01/10/2026

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Starting date 01/10/2026

PhD student: Simon BRIAND
Starting date 01/10/2026