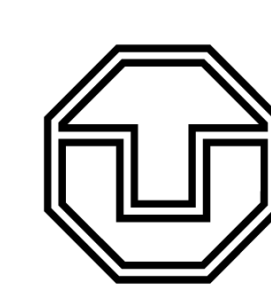


Molecular Brushes with Poly(2-oxazoline)-based Amphiphilic Diblock Copolymer Side Arms



TECHNISCHE
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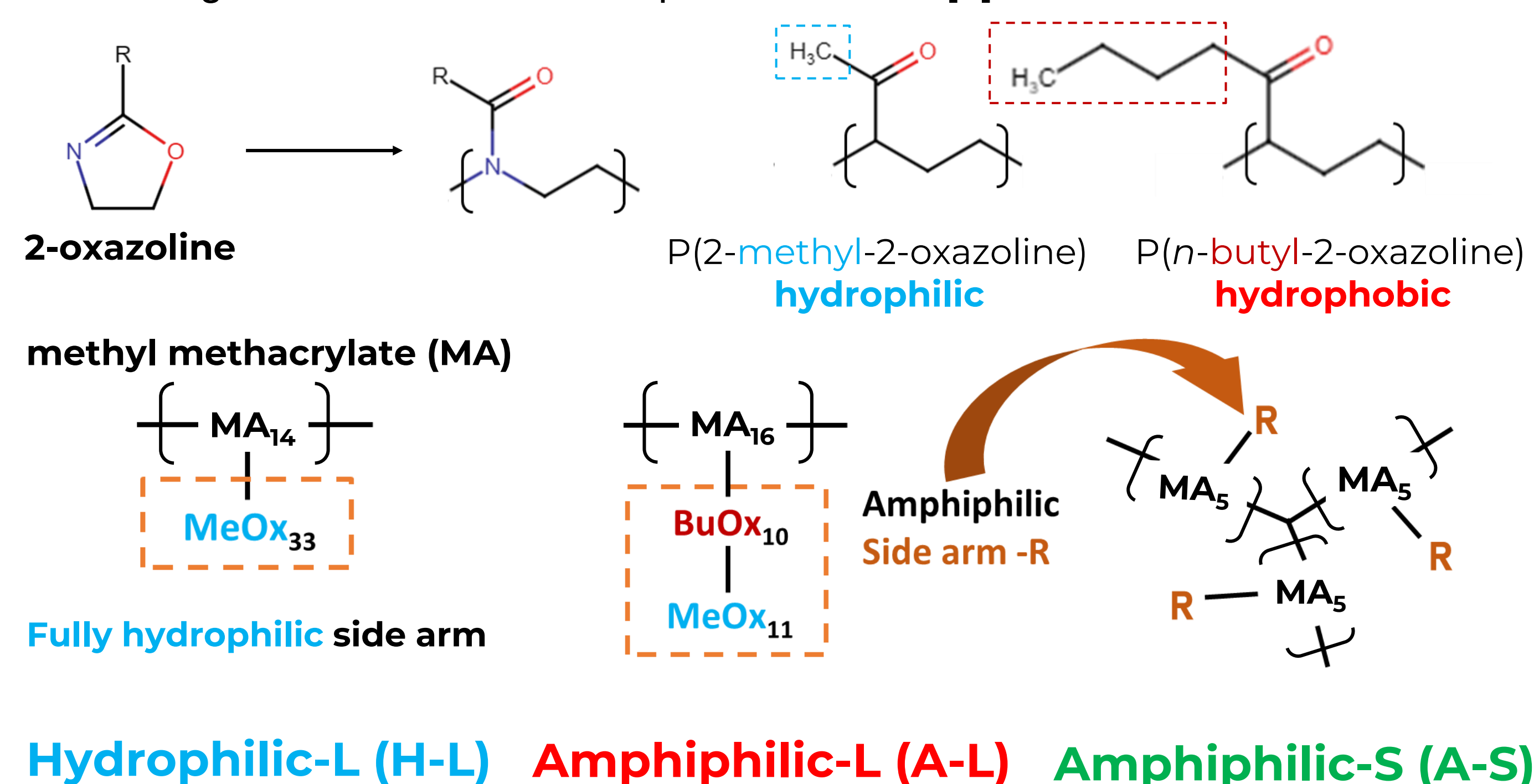
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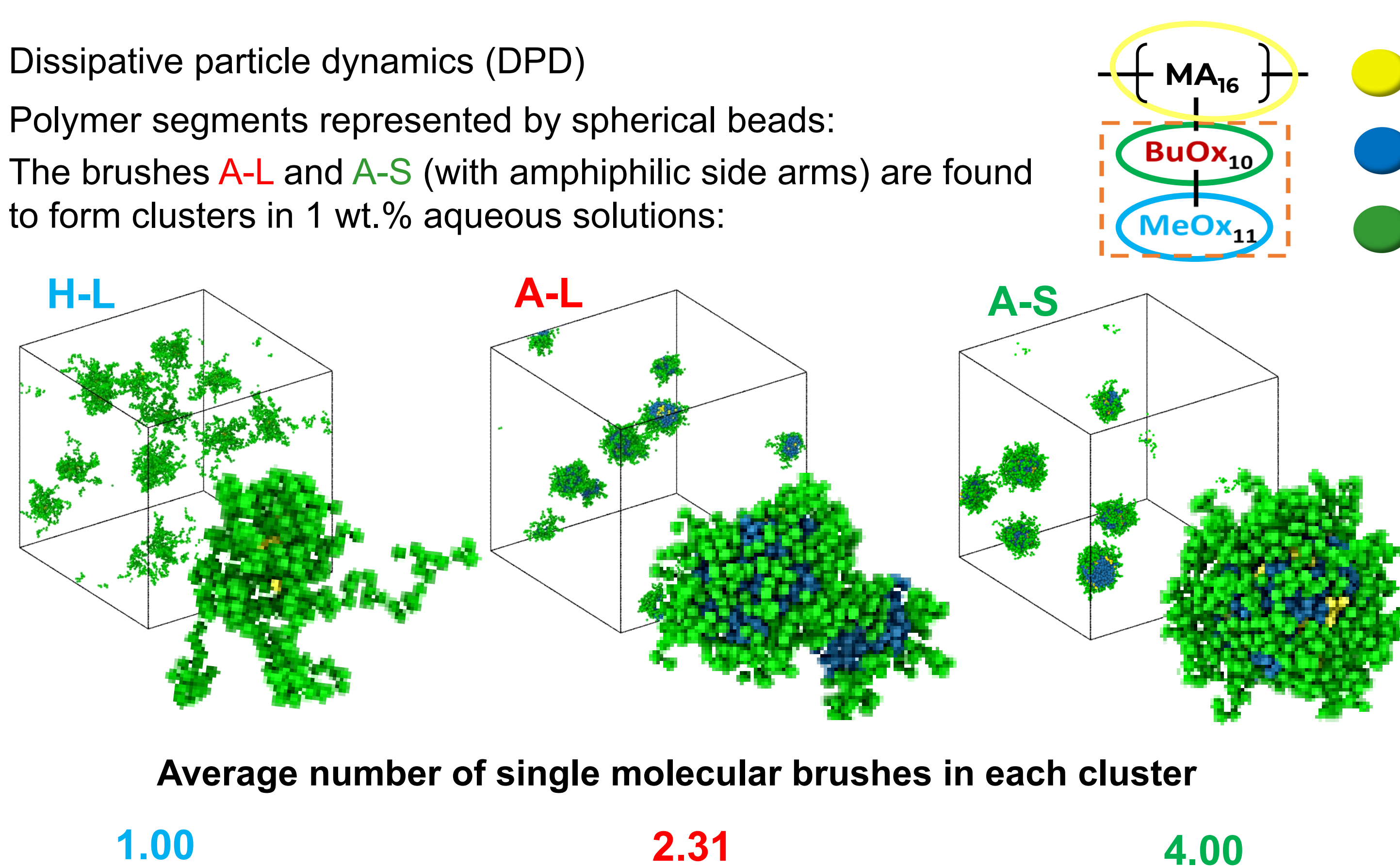
Sample information

- Poly(2-oxazoline)s (POx) are a class of non-toxic, biocompatible polymers [1].
- Molecular brushes with PMMA backbone and POx side arms are investigated focusing on their structures in aqueous solution [2]:



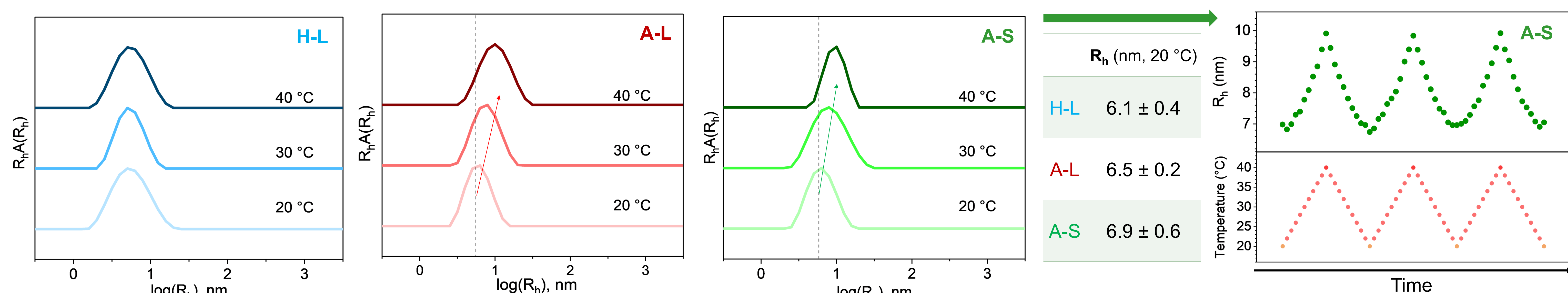
Simulation

- Dissipative particle dynamics (DPD)
- Polymer segments represented by spherical beads:
- The brushes A-L and A-S (with amphiphilic side arms) are found to form clusters in 1 wt.% aqueous solutions:



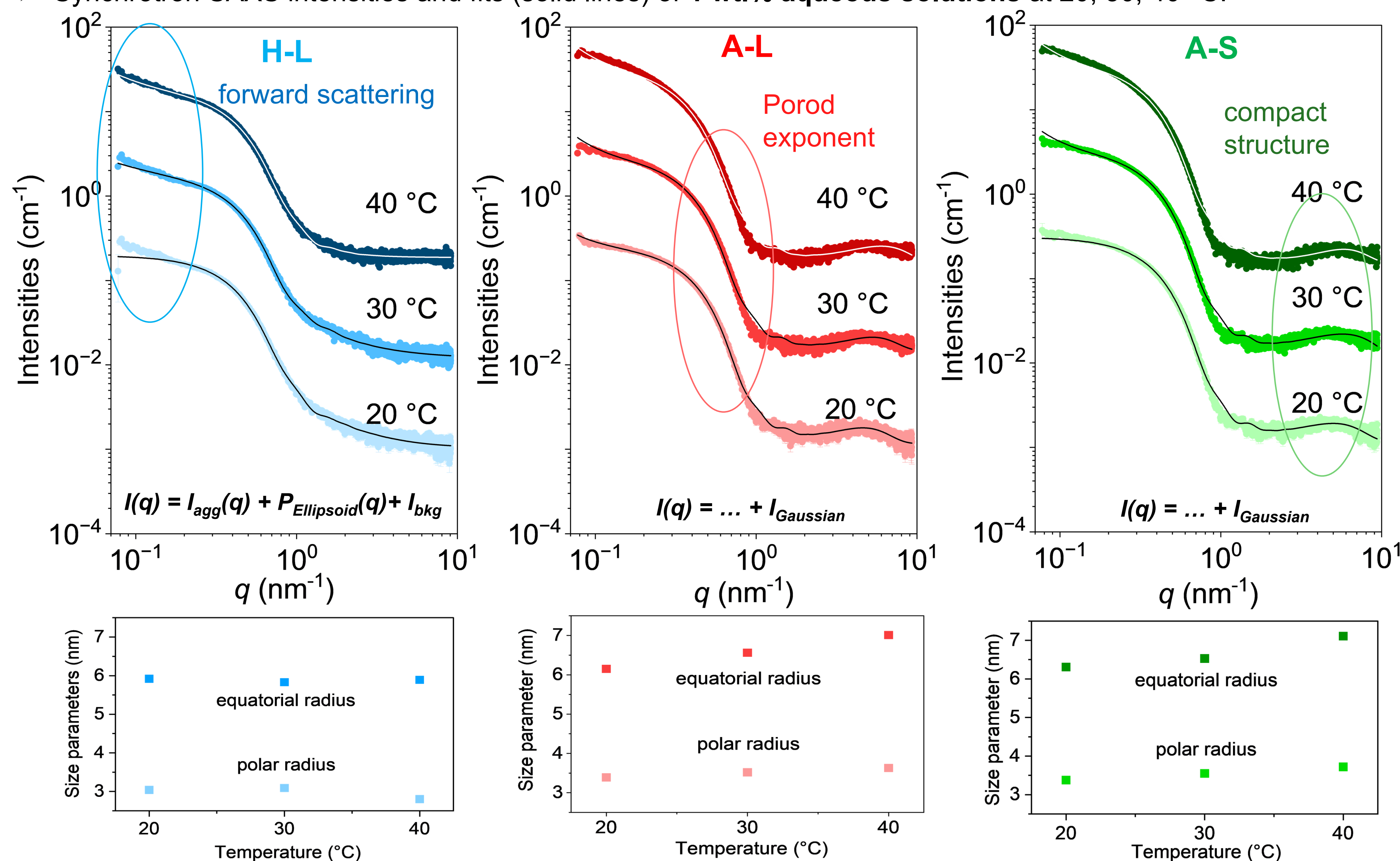
Dynamic Light Scattering

- Hydrodynamic Radius distributions in 1 wt.% aqueous solutions at 20, 30, 40 °C:
- DLS thermocycling of sample A-S shows the thermoresponsive transition is reversible:

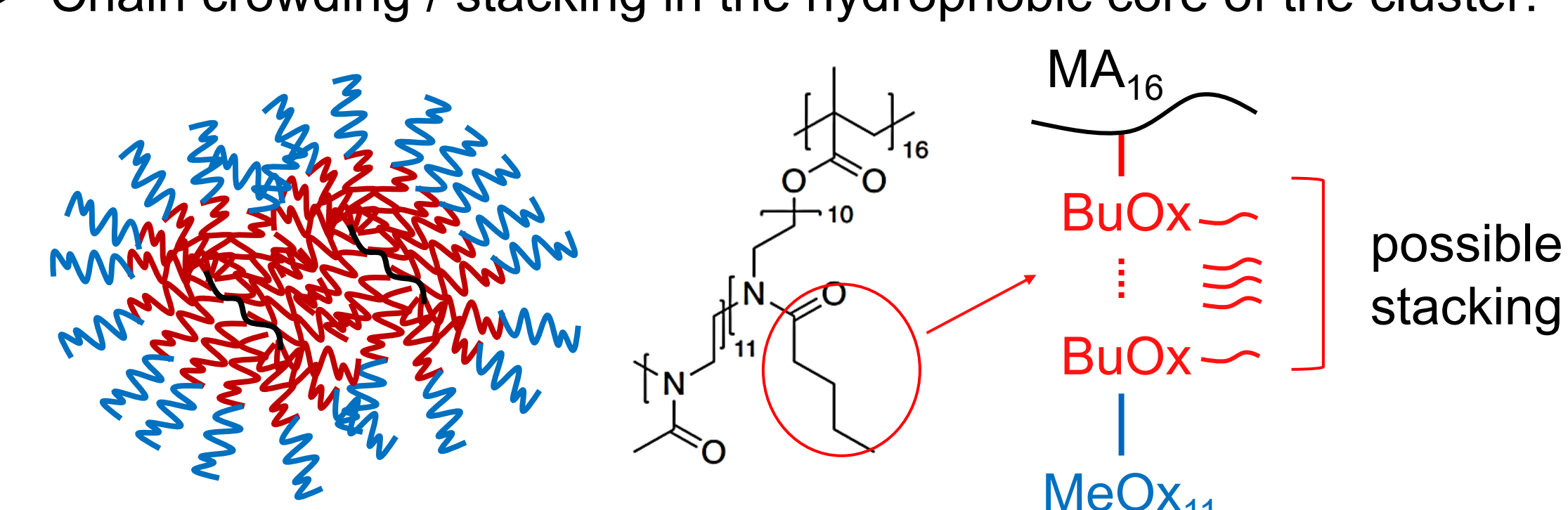


Synchrotron Small-angle X-ray scattering

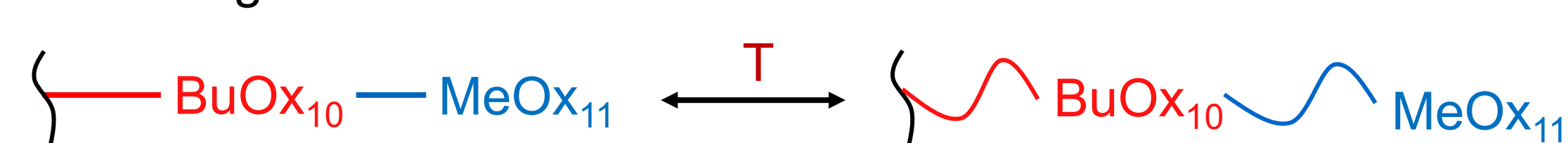
- Synchrotron SAXS intensities and fits (solid lines) of 1 wt.% aqueous solutions at 20, 30, 40 °C:



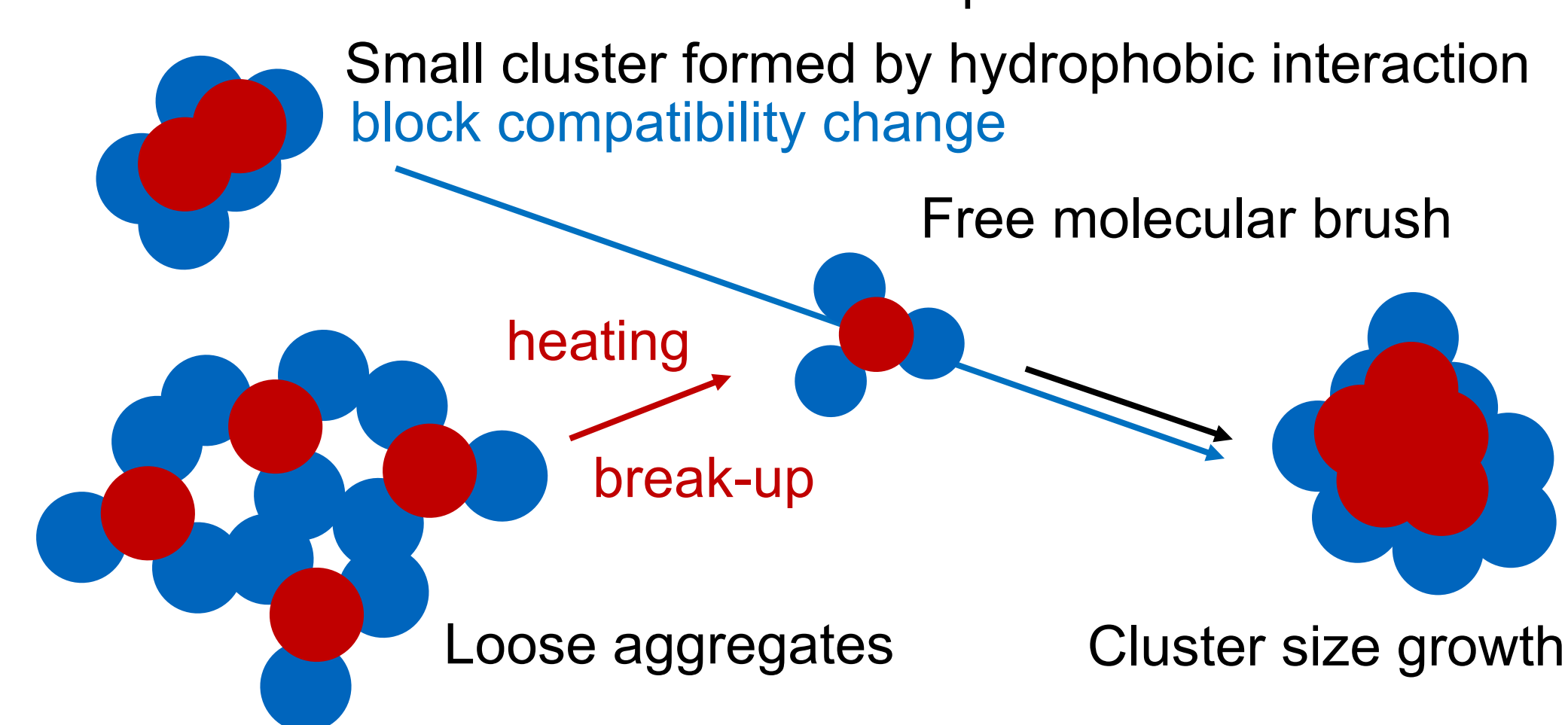
- Chain crowding / stacking in the hydrophobic core of the cluster:



- Temperature may affect the block compatibility (e.g., decrease of repulsive interaction), which leads to the observed structure rearrangement:



- Possible mechanism of the thermoresponsive behaviour:



Conclusions

- In 1 wt.% aqueous solution, the brush with hydrophilic side arm are ellipsoids with equatorial and polar radii of 6 and 3 nm.
- The brushes with amphiphilic side arms form small clusters via hydrophobic interactions of the BuOx core. The size of the cluster increases with temperature, possibly due to the decrease of repulsive interactions between BuOx and MeOx blocks [3].

References and Acknowledgments

- [1] R. Hoogenboom, *Eur. Polym. J.* **2022**, 179, 111521.
 - [2] J.-J. Kang, C. M. Papadakis et al., *Colloid Polym. Sci.* **2021**, 299, 193.
 - [3] L. Daoud, V. Lapinet et al., *Polymer Chemistry* **2024**, 15, 3641.
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