

# Molecular Design of Green Polymers for Fabric Surface Modification: A Multiscale Computer Simulation Approach

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# Project Overview

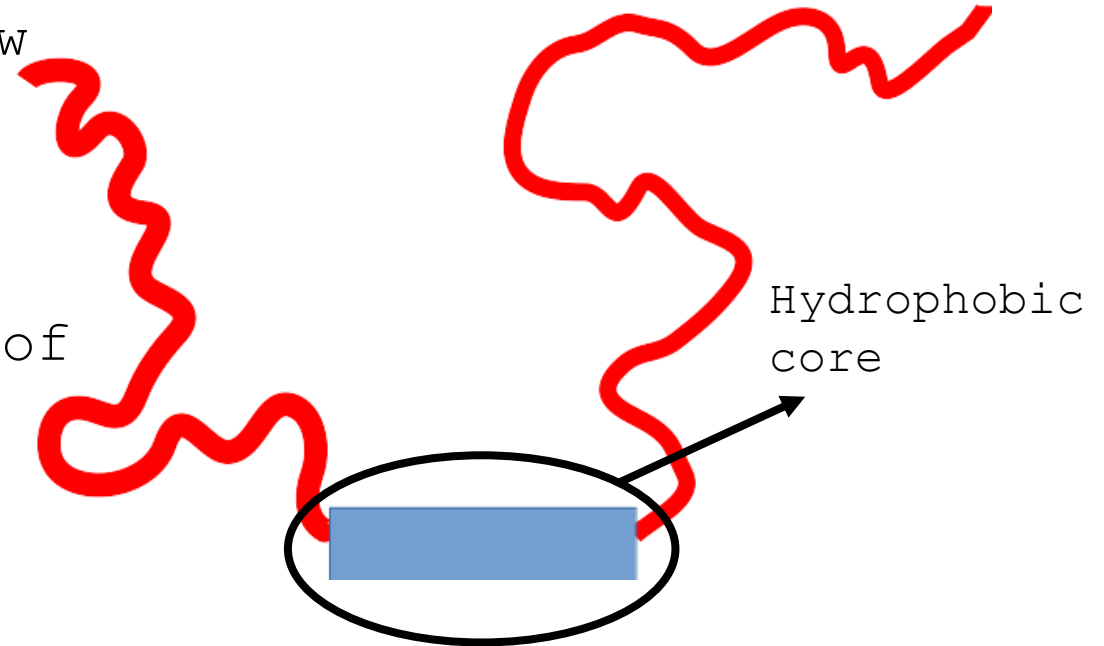
## Background

- SRPs (soil-release polymers) play a key role in fabric care formulations – coat fabric surface making it more stain resistant.
- Lower temperature washing cycles = reduced energy consumption.
- Commercial SRPs made using petroleum-sourced materials.

**Aim:** Develop a computational workflow for screening new greener SRPs.

## How?

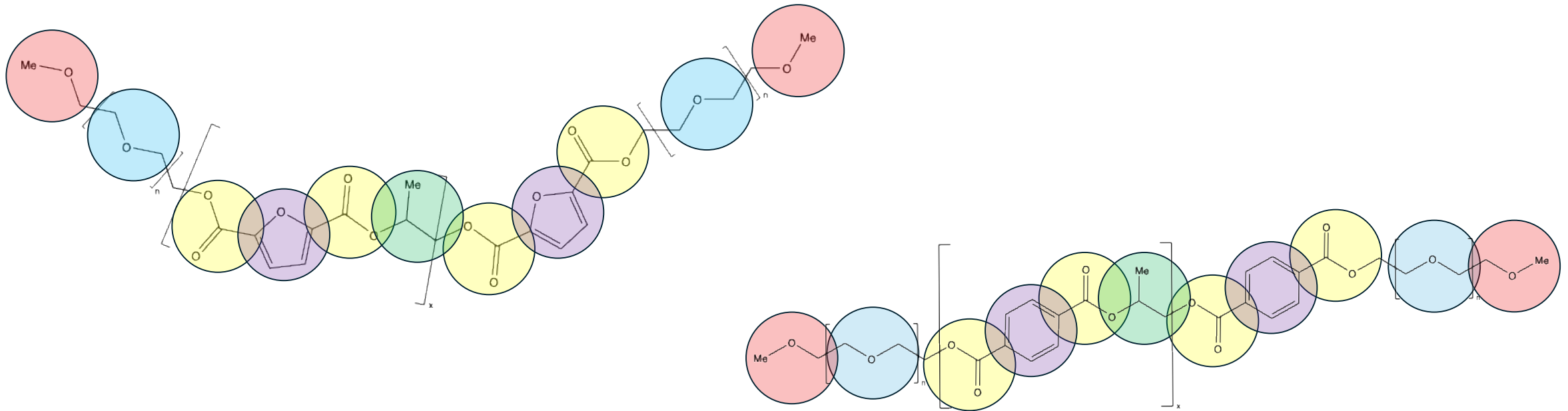
- Identifying the binding strength of the polymer to the surface.
- Accounting for aggregation behaviour and folding of the polymer in solution.



# Methods

## Set up

- Workflow developed based on 8 SRPs (2 linear, 6 branched) with 2 varying core components (commercial core and a ,better, greener core).



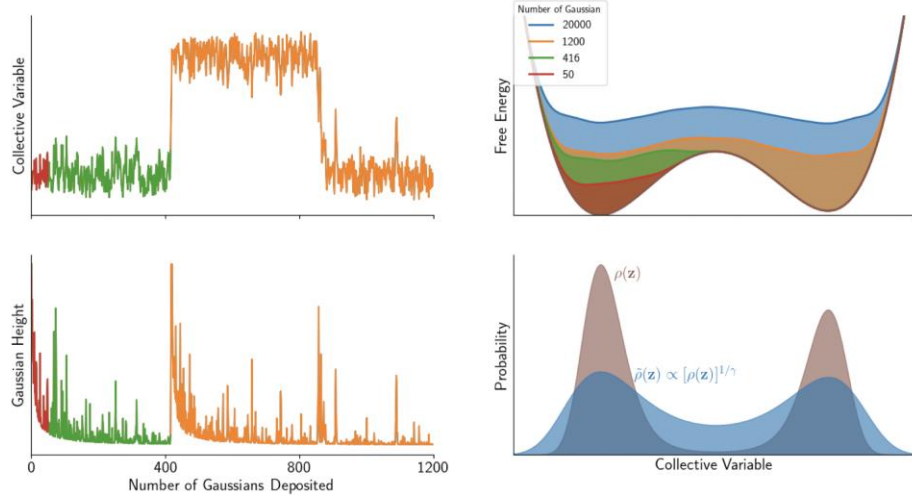
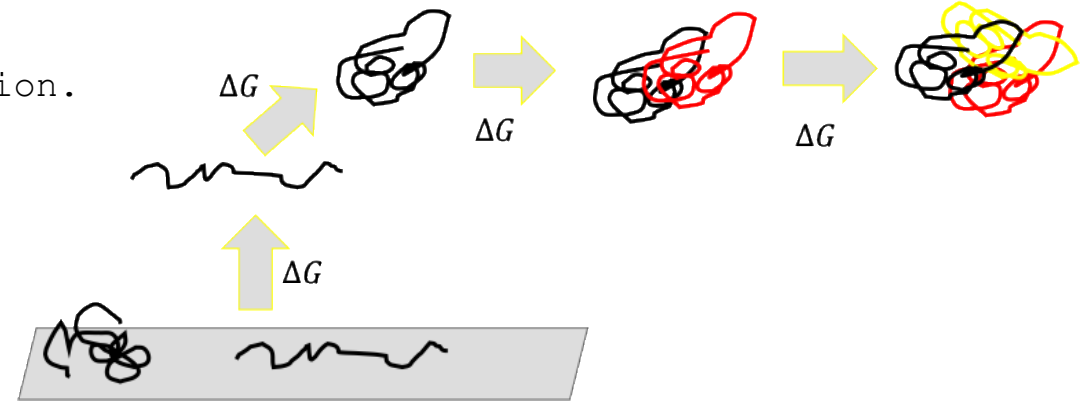
- High quality experimental observations<sup>1</sup> available that aided model development and validate results.

<sup>1</sup> Data acquired by the Mahon group at Durham University.

# Methods continued

1) 1 wt% solutions in water simulations via dissipative particle dynamics (DPD).

- Investigated aggregation in systems as big as ~30 polymers.
- Python cluster algorithm to analyse the aggregation in solution.
- Python code to extract hydrodynamic radii from simulations.



2) Well-tempered metadynamics simulations between 2 polymers.

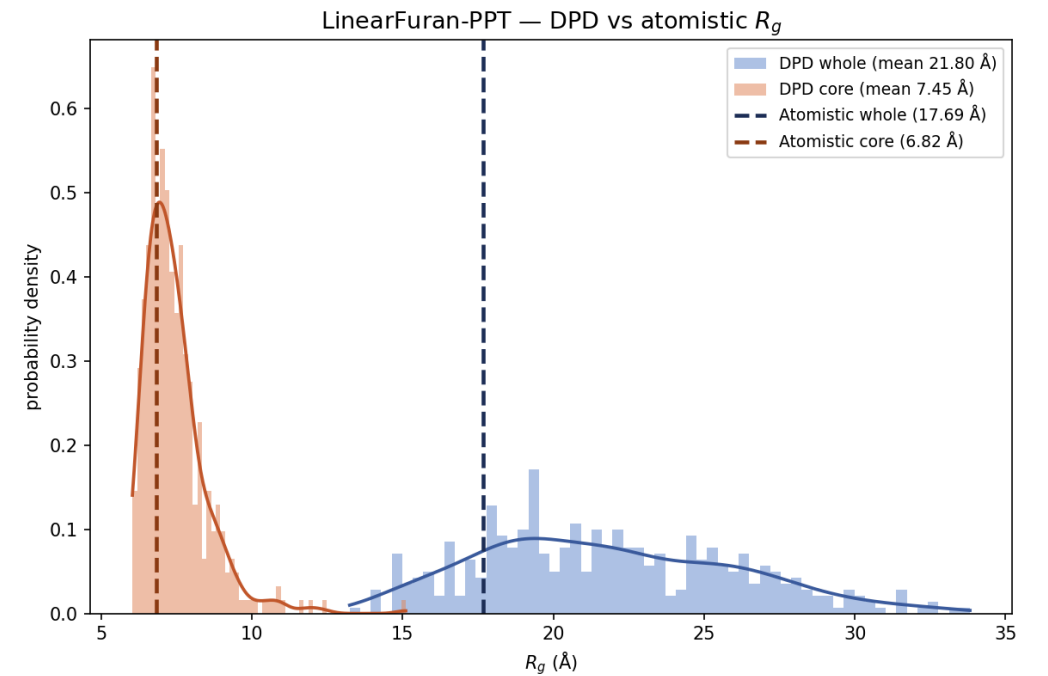
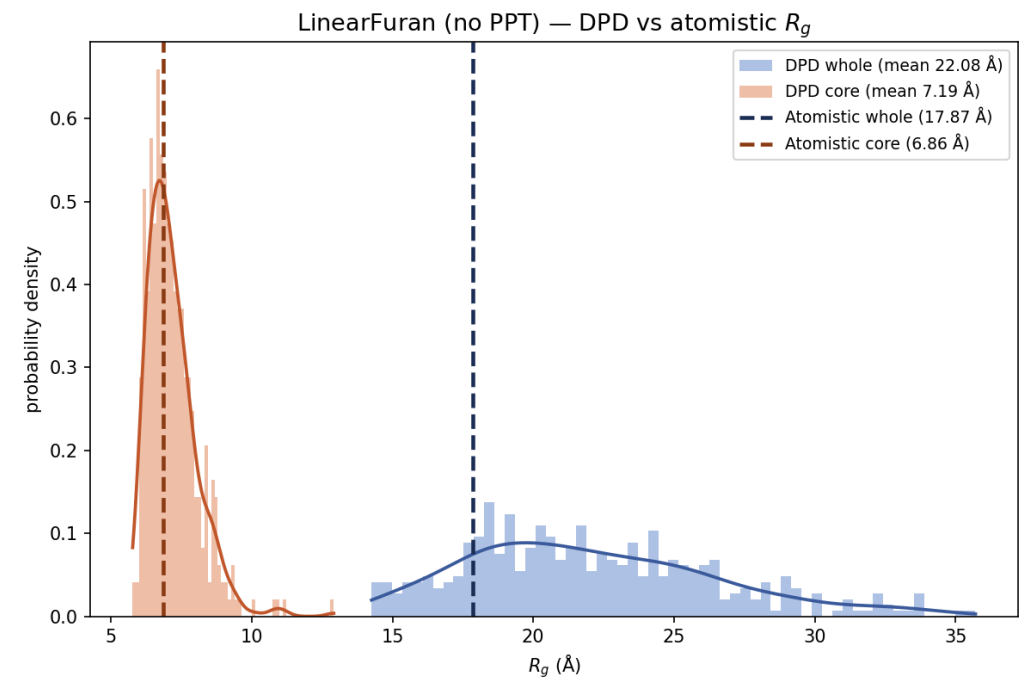
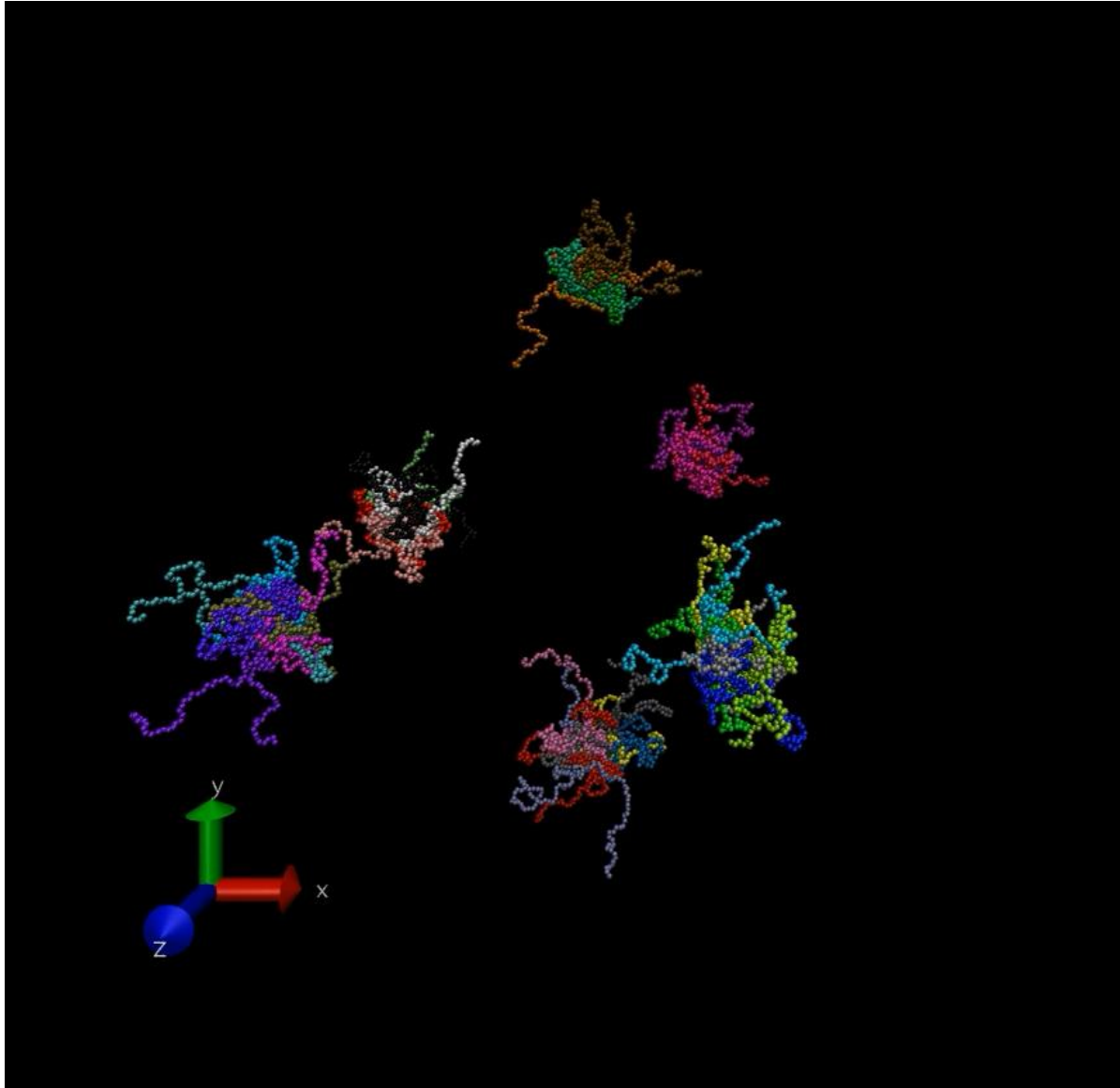
- Explored full free energy surface (FES) with the use of a bias.
- Python code used to extract free energy of dimerization from a FES.

Additionally:

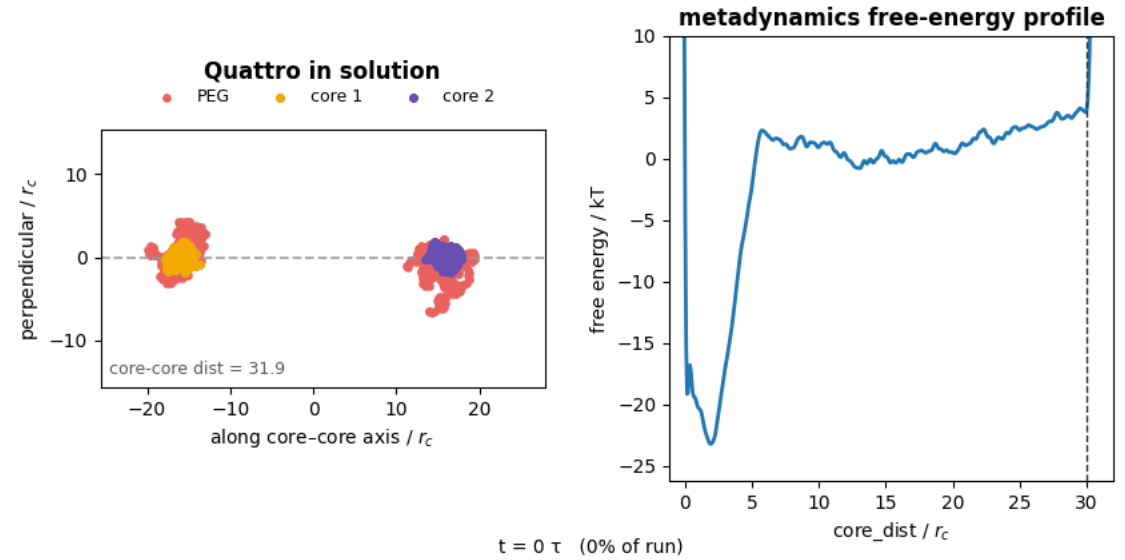
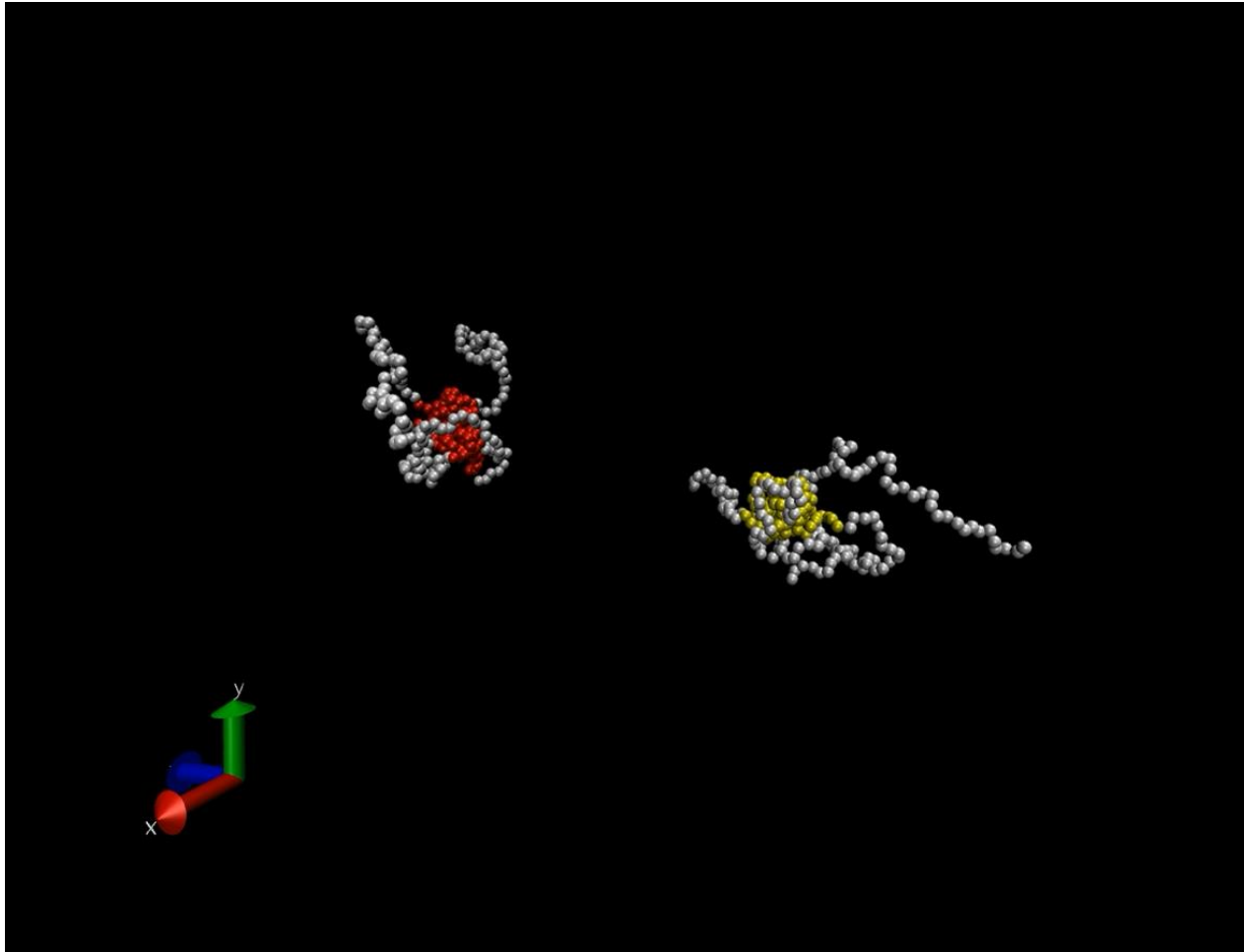
3) 1 polymer in solution simulations via DPD.

- Investigated molecule sizes compared to reliable atomistic molecular dynamics (MD) simulations.

# Results



# Results cont.



|               | Surface / kT | Dimer / kT |
|---------------|--------------|------------|
| Linear Furan  | ~1           | 2          |
| Linear PPT    | 3            | 10         |
| Tristar       | 18           | 24         |
| Tristar-PPT   | 32           | 26         |
| Tetrastar     | 32           | 35         |
| Tetrastar-PPT | 27           | 37         |
| Quattro       | 18           | 23         |
| Quattro-PPT   | 18           | 41         |

# Discussion and Conclusions

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- Polymer angle stiffness and thermodynamics played a big role in correct model parametrization.
- Commercial core is more likely to aggregate compared to the proposed greener core for the same architecture.
- As branching increases, so does the dimerization free energy which hinders surface absorption and therefore the key factor contributing to underperformance of an SRP core.

## **Next steps:**

- Combine workflow developed for aggregation in solution with surface absorption workflow.
- Wider application of our workflows in formulation chemistry.

# Thank You For Listening!

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