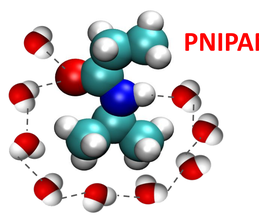
Studying conformations of dextran-conjugated thermosensitive bottlebrush polymers

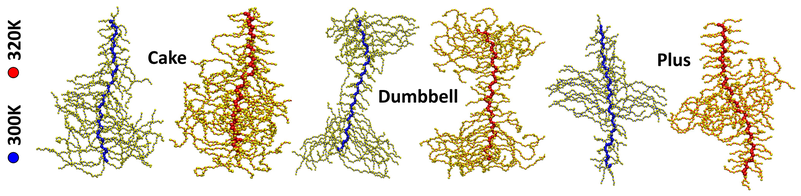
Soumil Y. Joshi, Parisa Farzeen, and Sanket A. Deshmukh*
Department of Chemical Engineering, Virginia Tech, Blacksburg, 24060
sanketad@vt.edu

GlycoMIP NSF Materials Innovation Platform

Prior Work

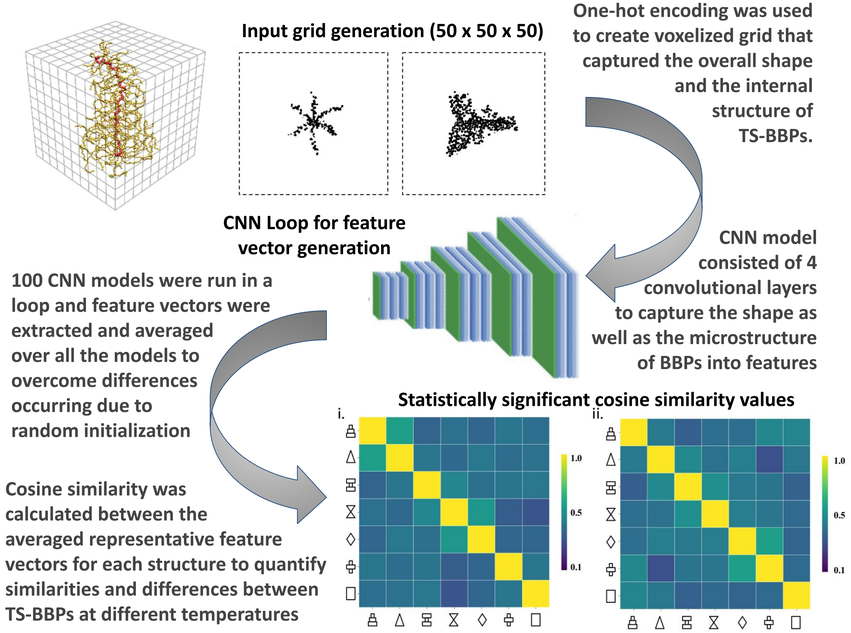
- Effect of shape on conformations of soft materials like bottlebrush polymers (BBPs), is not well understood due to their softness and flexibility. Here, **molecular dynamics** helps.
- BBP conformations can also be influenced by using thermosensitive polymers as BBP side chains and the temperature.
- Varying the arrangement and lengths of side chains, different shapes of BBPs were simulated.
- It was observed that the arrangement of side chains along the TS-BBP backbone and their immediate environments dictate the compactness and bending in these architectures.





Similarity quantification using Convolutional Neural Network

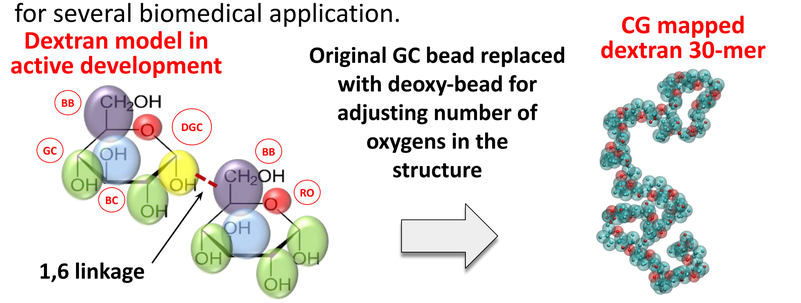
- CNNs can analyze flexible objects very well due to their ability to identify shapes irrespective of their orientation, something essential for soft-matter architectures.



Link: https://doi.org/10.1038/s41524-022-00725-7

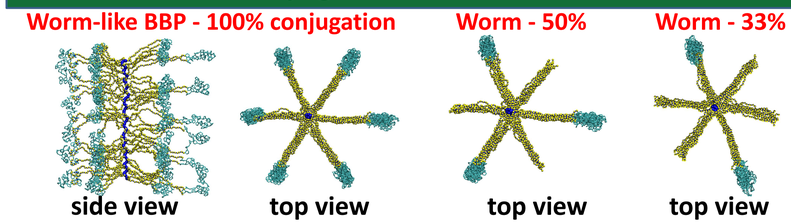
Dextran model development

- PNIPAM-Dextran copolymers and architectures have shown potential for several biomedical application.

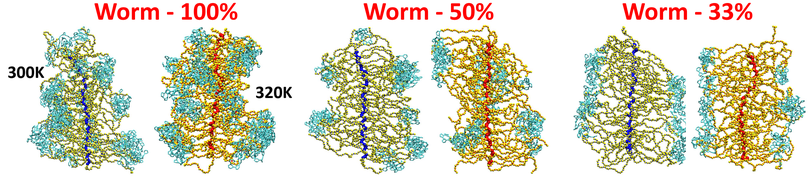


- In-depth investigation of conjugated non-cylindrical BBPs could help understand relationships between conjugate groups and BBP shapes.

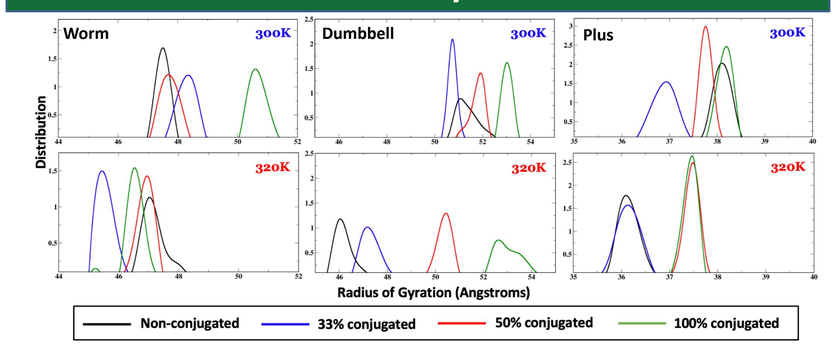
Dextran-conjugated thermosensitive BBPs



- Simulations run at 300 K and 320 K (below & above LCST of PNIPAM)

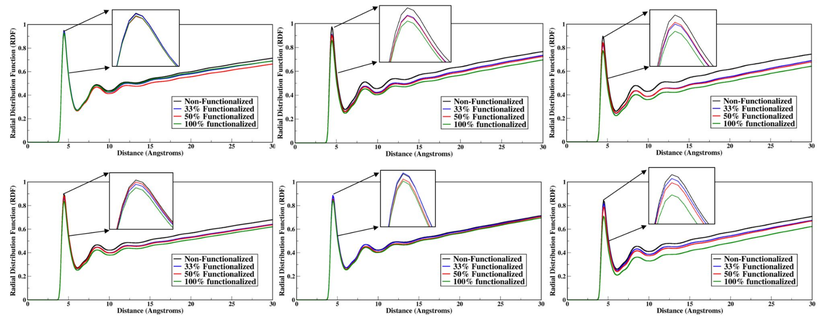


Radius of Gyration



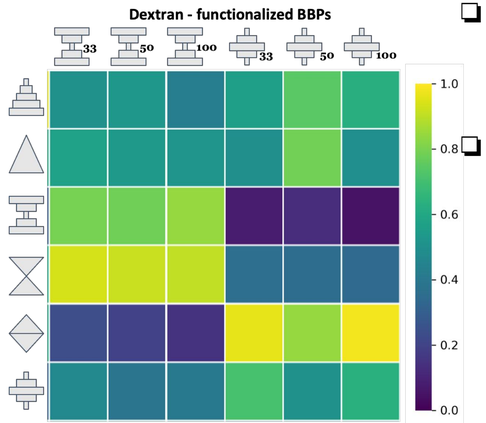
- In most cases, R_g increased with dextran conjugation
- Correlation with non-conjugated BBP was different for different shapes and temperatures

Structure of solvent



- Little change in hydration shell structures in case of Worm-like BBP
- Considerable change was observed in the RDF for Dumbbell at 300K but not at 320K
- Significant changes at both 300K and 320K for the Plus-like structure

Insights from CNN



- Higher similarity between conjugated dumbbell-like structures and hourglass-like BBPs
- Conjugated plus-like BBPs also show higher similarity with gradually changing diamond-like structures

Dextran conjugation results in BBP conformations such that interfaces between different layers get hidden

References and Acknowledgements

[1] Radzinski, S. C.; Matson, J. B; et. al. ACS Macro Letters, 2017, 6, 1175–1179.
[2] S. Y. Joshi, S. Singh and S. A. Deshmukh, npj Comput. Mater., 2022, 8, 45
[3] Bejagam, K. K.; et. al. Phys. Chem. Lett., 2018, **9**, 6480–6488

This work was supported by GlycoMIP, a National Science Foundation Materials Innovation Platform funded through Cooperative Agreement DMR-1933525.

NERSC
VIRGINIA TECH Advanced Research Computing
Computational Design of Hybrid Materials (CDHM)