Trainee Research Highlight

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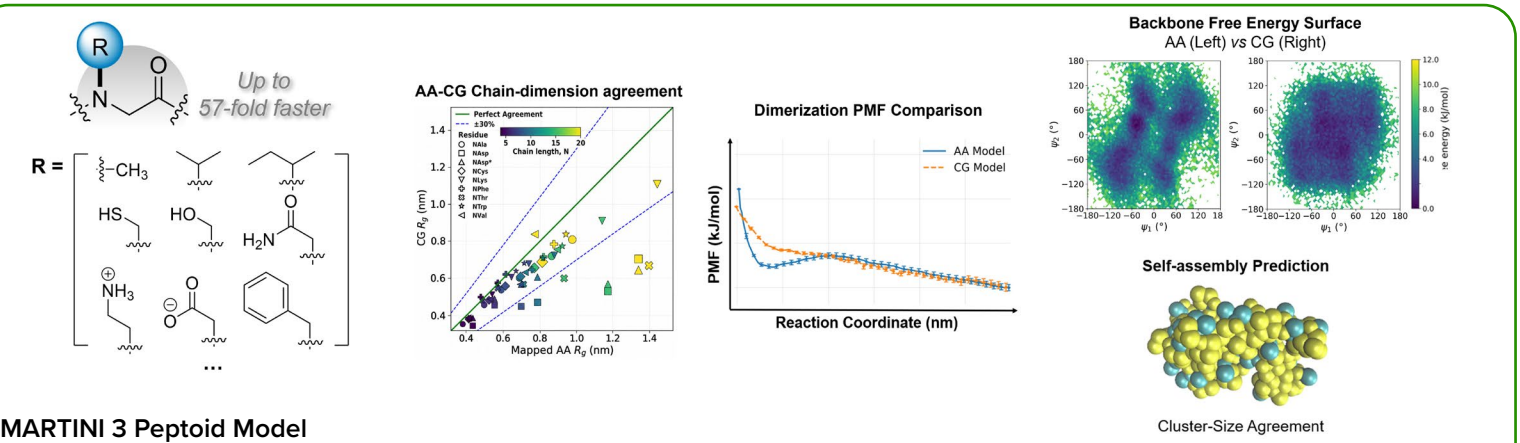
Extending the MARTINI 3 Coarse-Grained Force Field to Polypeptoids

Wang, J., Yu, Z., Zhao, M., *Journal of Chemical Theory and Computation*, ASAP (2026).



MARTINI 3 Peptoid Model
Overview of the MARTINI 3-compatible coarse-grained peptoid model developed for 19 commonly used residue types. The model was validated against atomistic reference simulations across chain dimensions, conformational free-energy landscapes, dimerization thermodynamics, and self-assembly behavior, while achieving up to a 57-fold increase in computational efficiency.

Scientific Achievement:

Peptoids are attractive to the materials and biomolecular communities because their side-chain chemistry and sequence can be precisely controlled. However, correlating molecular sequence to larger-scale behavior such as folding, aggregation, membrane interactions, and nanostructure formation remains computationally challenging. In this work, we developed the first MARTINI 3-compatible coarse-grained force field for polypeptoids, covering 19 commonly used residue types. The model was parametrized from all-atom simulations and validated against atomistic benchmarks, including chain dimensions, backbone conformational behavior, dimerization free energies, and multi-chain aggregation. To support broad community use, the parameters and workflow were integrated into martinize2, enabling automated generation of MARTINI 3 peptoid structures and topologies. This model provides a transferable and efficient framework for studying large-scale sequence-structure-assembly relationship in peptoid science.

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Why is this paper significant?

"Peptoids are highly tunable, sequence-defined materials, but their conformational flexibility and slow backbone isomerization make large-scale atomistic simulations computationally challenging. We believe this work provides an important step toward bridging molecular-level understanding and mesoscale peptoid behavior. By combining improved computational efficiency with compatibility with the MARTINI 3 framework and automated topology generation through martinize2, we hope this model will enable broader studies of peptoid conformations, self-assembly, membrane interactions, and nanostructure formation, and ultimately support the rational design of functional peptoid-based materials."

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