

Can Cyclic Polypeptoids with Oppositely Charged End-Group Aggregate in Solution?

Scientific Achievement

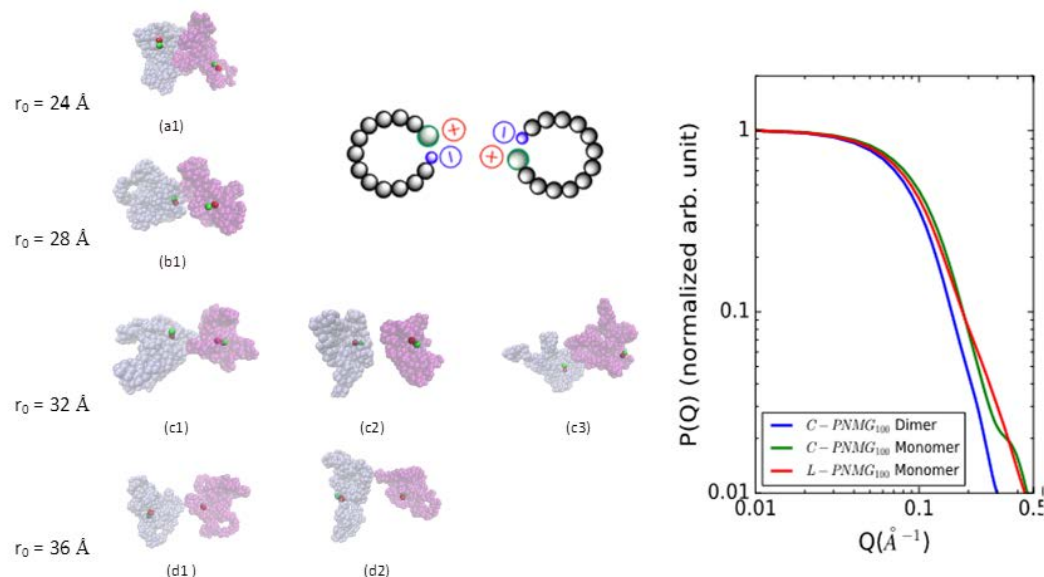
Answered the question of *whether* cyclic peptoids (a class of biomimetic polymers) with oppositely charged end-groups can aggregate in solution and *why*.

Significance and Impact

Dynamic aggregation of polymers can result from a competition between forces that favor aggregation (e.g., dipole-dipole interactions and solvophobic effects) and those that oppose it (e.g., the need for the dipoles/charged ends to be solvated). These fundamental studies are relevant to understand and optimize self-assembly of soft-matter systems as well as utilize these biomimetics.

Research Details

- Cyclic polypeptoids bearing oppositely charged chain ends form small dynamic clusters in dilute alcohol solution
- The cluster formation is driven by complex interplay of various secondary interactions dipole-dipole interaction, solvophobic effect, solvation of dipole)
- Linear polymer analogs, in the absence of the corresponding dipole-dipole attraction, failed to form clusters



Du, P.; Li, A.; Li, X.; Zhang, Y.; Do, C.; He, L.; Rick, S., John, V. J.; Kumar, R.* and Zhang, D.* MD simulation snapshots showing the cluster formation of cyclic polypeptoids and the relevant simulated SANS profiles
Phys. Chem. Chem. Phys. **2017**, DOI: 10.1039/C7CP01602F.