Cyclic Polymers Form Dynamic Clusters in Solution Due to A Delicate Balance of Secondary Interactions

Scientific Achievement

It was revealed that secondary interactions encoded in the molecular architecture (i.e., cyclic versus linear) can confer control over the formation of dynamic intermolecular assemblies.

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 *Phys. Chem. Chem. Phys.* **2017**, DOI: 10.1039/C7CP01602F. cyclic polypeptoids and the relevant simulated SANS profiles









