Scientific Achievement
Combining computational, theoretical and experimental approaches, this study shows how modulating hexamer-hexamer interactions and component stoichiometric ratio can result in different microcompartment morphologies.

Significance and Impact
This work develops a multi-scale computational approach to study how amino acid mutations alter hexamer-hexamer interactions and control the assembly morphology. The findings will help guide future studies to assemble specific BMC structures with desired functionality.

Research Details
- We first use all-atom molecular dynamics (AAMD) simulation to determine the interaction strength and bending angles between hexamers. Then from AAMD simulation, we construct a coarse-grained model to study the assembly morphology.
- We compare the assembly morphology with experimental data and determine how mutations of amino acids can alter the assembly shapes.
- Using CG simulation and thermodynamic models, we also determine the role of stoichiometric ratio of the three major component proteins in microcompartments and explore how modulating protein interactions can regulate the assembled morphology.

Yaohua Li, Nolan W. Kennedy, Siyu Li, Carolyn E. Mills, Danielle Tullman-Ercek, and Monica Olvera de la Cruz. ACS Central Science (2021).

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