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PointNet-meso: A Tool for Detecting Self-Assembled Block Oligomer Morphologies

Intellectual Merit

block oligomer Screening chemistry and architecture through molecular simulations to for promising candidates find functional effective materials requires morphology identification techniques. Common strategies for structure identification include structure factors and order parameters, but these fail to identify imperfect structures in simulations with incorrect system sizes.

We developed a machine learning approach, PointNet-meso, for called mesophase classification different including network morphologies (double gyroid, single gyroid, double diamond, and plumber's nightmare). The trained PointNet-meso model achieves an accuracy as high as 0.99 for globally ordered morphologies formed by linear diblock, linear triblock, and 3-arm and 4-arm star block oligomers, and it also allows for the discovery of emerging ordered patterns from non-equilibrium systems.

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Z. Shen, Y. Z. S. Sun, **T. P. Lodge** & **J. I. Siepmann**, *J. Phys. Chem. B*, **(2021)** DOI: 10.1021/acs.jpcb.1c02389

