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RESCHEDULED Identifying polymer states by machine learning

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The ability of a feed-forward neural network to learn and classify different states of polymer configurations is systematically explored. Performing numerical experiments, we find that a simple network model can, after adequate training, recognize multiple structures, including gas-like coil, liquid-like globular, and crystalline anti-Mackay and Mackay structures produced from Monte Carlo simulations. The network can be trained to identify the transition points between various states, which compare well with those identified by independent specific-heat calculations. Our study demonstrates that neural network provides an unconventional tool to study the phase transitions in polymeric systems. The direct use of molecular coordinates as input into the network underlies the robustness and simplicity of our approach, and suggests that other simulation tools, such as molecular dynamics, could be incorporated as well. The outcome of this work provides a compelling reason to incorporate machine learning techniques into molecular simulations more generally, as a powerful hybridized computational tool for the future study of soft-matter systems.

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