







Special Issue Reprint

Scientific Machine Learning for Polymeric Materials

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Polymeric materials play a key role in supporting the ever-increasing demand for electronics. medicines, plastics, sensors, and the transition to renewable energy sources. This is achieved through polymers' distinct features at different structural and temporal scales (i.e., a subtle change in their atomic or mesoscopic structures leads to a totally emergent functionality). However, the design of new polymeric materials is still a lengthy process. This major challenge is related to their inability to comprehensively bridge phenomena that occur at temporal scales from tens of nanoseconds to seconds or spatial scales from nanometers to meters. Indeed, scientific datasets in this field are sparse and include only directly observable quantities, while the underlying processes are either too complex to observe directly or are completely unknown. To move towards an accelerated on-demand design for polymeric materials, recent breakthroughs in scientific machine learning (SciML) can be leveraged to explore the interactions of physics at different spatial and temporal scales. This reprint presents scientific works on SciML—e.g., physics-guided neural networks, physics-informed neural networks, physics-encoded neural networks, and neural operators—for multi-scale multi-temporal structures and mechanisms with polymer behaviors (rheology, self-assembly, phase transition, etc.).





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