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Water Diffusivity in Amorphous Epoxy Resins: An Autonomous Basin Climbing-Based Simulation Method

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Abstract : Epoxy-based materials are frequently exposed to high-humidity environments in many engineering applications. As a result, their material properties would be degraded by water absorption. A full characterization of the material properties under hygrothermal conditions requires time- and cost-consuming experimental tests. To gain insights into the physics of diffusion mechanisms, atomistic simulations have been shown to be effective tools. Concerning the diffusion of water in polymers, spatial trajectories of water molecules are obtained from molecular dynamics (MD) simulations allowing the interpretation of diffusion pathways at the nanoscale in a polymer network. Conventional MD simulations of water diffusion in amorphous polymers lead to discrepancies at low temperatures due to the short timescales of the simulations. In the proposed model, this issue is solved by using a combined scheme of autonomous basin climbing (ABC) with kinetic Monte Carlo and reactive MD simulations to investigate the diffusivity of water molecules in epoxy resins across a wide range of temperatures. It is shown that the proposed simulation framework estimates kinetic properties of water diffusion in epoxy resins that are consistent with experimental observations and provide a predictive tool for investigating the diffusion of small molecules in other amorphous polymers.

Keywords : epoxy resins, water diffusion, autonomous basin climbing, kinetic Monte Carlo, reactive molecular dynamics
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