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Investigation of the effects of methanol presence on characteristics of sulfonated aromatic electrolyte membranes: Molecular dynamics simulations

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Highlights

- SPPO membranes of different methanol concentrations were studied by MD simulation.
- SPPO membranes show phase separation on the uptake of methanol.
- Sulfonic acid groups were solvated more with water compared to methanol solvent.
- Larger solvent clusters formed at lower methanol concentrations.
- Methanol diffusion coefficient increased with increasing methanol concentration.

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