Interfacial Structure and Thermal Transport in Polymer-Grafted Nanoparticle Nanofluids: A Molecular Dynamics Study

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Nanofluids, composed of nanoparticles dispersed in a base liquid, have attracted considerable attention as advanced heat transfer media due to their enhanced thermal conductivity. However, their practical application is hindered by nanoparticle agglomeration and sedimentation, which compromise long-term dispersion stability. To overcome this limitation, nanofluids based on polymer-grafted nanoparticles (PGNPs), where polymer chains are tethered to the nanoparticle surface, have been proposed[1]. PGNPs exhibit superior dispersion stability and are also expected to enhance interfacial heat transport[2,3]. Nevertheless, the mechanisms by which the polymer shell structure and the surrounding ordered solvent layer (nanolayer) jointly influence thermal conductivity remain unclear.

In this study, molecular dynamics (MD) simulations were performed to investigate the relationship between interfacial structure and thermal transport properties in PGNP-based nanofluids at the molecular scale. The grafting density of polymer chains and the intermolecular interaction energy were systematically varied to examine their effects on polymer conformations, solvent structuring near the interface, and overall thermal conductivity.

The results indicate that thermal conductivity exhibits a strong dependence on intermolecular interaction energy at high grafting densities: it increases significantly with stronger interactions, whereas it decreases under weaker interactions. Heat-flux decomposition shows that solvent–solvent energy transport dominates at low grafting densities, whereas polymer–polymer and polymer–solvent contributions become increasingly important at higher grafting densities. Additionally, weaker interpolymer interactions enhance the overlap between polymer and solvent density distributions, thereby facilitating interfacial energy transport.

These findings highlight the critical role of interfacial structure in governing heat transport in PGNP nanofluids and provide molecular-level insights for designing high-performance nanofluids.

Keywords:
Nanofluids, Interfacial molecular layer, Molecular dynamics, Thermal conductivity

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