INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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In the past decade, multilayered graphene oxide (GO) membranes have emerged as promising candidates for desalination and wastewater treatment applications. Despite their potential, a comprehensive understanding of separation mechanisms remains elusive due to the intricate morphology and structural arrangement of interlayer galleries. This thesis addresses these challenges by constructing two distinct structural configurations, namely lamellar and non-lamellar, to investigate separation mechanisms at the atomistic level. Moreover, one major issue with layered GO membranes is their tendency to swell in an aqueous environment. Recognizing the tendency of layered GO membranes to swell in aqueous environments, this thesis explores cation intercalation within interlayer galleries as a promising solution to mitigate this problem. The applicability of lamellar, non-lamellar, and cation-intercalated GO membranes as forward osmosis (FO) and reverse osmosis (RO) membranes in separation and purification applications is studied using non-equilibrium molecular dynamics (MD) simulations. Real-life scenarios, including seawater, pharmaceutical industrial wastewater, shale gas wastewater, and human urine are considered to assess the performance of GO membranes. These GO membranes exhibit an improved trade-off between water permeance and selectivity compared to conventional polymeric membranes. This enhanced performance is attributed to the inherent structural characteristics of GO membranes, such as nanosized 2D channels and open edges, which enable the rapid movement of water molecules across membrane layers while efficiently retaining undesired species. Additionally, the nanosized GO nanosheets have abundant oxygen-containing functional groups (OFGs), enhancing their mechanical strength and chemical stability.