

# Monolayer graphene membrane for high-temperature organic solvent nanofiltration in harsh solvents

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## Abstract:

Separation, purification and recovery of organic solvents play a key role in the pharmaceutical, chemical and petroleum industries. Organic solvent nanofiltration (OSN), which applies membranes for molecular-level separations from organic solvents, is an environmentally friendly method that requires less footprint. However, one of the main barricades of OSN is the instability of membranes that struggle to fulfill some industrial operating conditions with high temperature in harsh solvents. Monolayer graphene demonstrates atomic thickness combined with remarkable mechanical strength, excellent resistance to organic solvents and high temperature, offering new possibilities for high-temperature OSN. In this presentation, I will discuss our research on molecular transport across monolayer graphene membrane via molecular dynamics simulations and resistance model to guide the design of defect-tolerant graphene composite membrane. With both pore size and permeance taken into consideration, we engineered crosslinked P84 polyimide (PI) substrate to enable nanoporous graphene membranes for high-temperature OSN in harsh solvents. The crosslinked P84 polyimide (PI) substrate could effectively mitigate the impacts of leakage on graphene to allow selective transport without defect sealing. The resultant graphene membrane showed a rejection of 92.7% to Rose Bengal ( $1017.64 \text{ g mol}^{-1}$ ) in ethanol, and constant rejection ( $\sim 90\%$ ) of Allura Red AC ( $496.42 \text{ g mol}^{-1}$ ) in harsh polar solvent N, N-dimethylformamide (DMF) at  $100^\circ\text{C}$  for 10 days. This work may open new opportunities for industrial separation in organic solvents at high temperature and accelerate the realization of full potential of the graphene.

This research was done in collaboration with Dr. Liling Zhang, from Institute for High Performance Computing, ASTAR, Singapore, Dr. Liang Shen and Prof. Sui Zhang, from National University of Singapore, Singapore, Prof. Wei Liu, from Southeast University, Nanjing, and Prof. Rohit Karnik, from Massachusetts Institute of Technology, Cambridge, Massachusetts, United States.

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