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# Water permeation in polymeric membranes: Mechanism and synthetic strategy for water-inhibiting functional polymers

Yusuke Araki[a], Yusei Kobayashi[a], Touru Kawaguchi[b], Takashi Kaneko[b], Noriyoshi Arai[a,*]

[a] *Kindai University, 3-4-1, Kowakae, Higashi-Osaka, Osaka, Japan*
[b] *Advanced Research and Innovation Center, DENSO CORPORATION, Nisshin, Aichi, Japan*

**Abstract**

The prediction and control of penetration in a polymeric membrane is of critical importance in green chemistry and energy technology, including gas separation, water purification, and desalination. We performed molecular simulations of water transport through a polymeric membrane to clarify the key factors that dominate water permeation. The effects of additives and chemical interaction (solubility) on water inhibition were investigated. We found that additives reduce water permeability into the membrane. Upon incorporation of the additive, strength of coordination of water molecules near the membrane surface increases. Thus, the penetration frequency of water molecules into the membrane decreases. It is suggested that the local environment near the membrane surface plays a significant role in controlling water permeability. In order to gain deeper insights into the polymer design, we discussed the chemical interaction (solubility) parameter change between polymer chains and additives. Using a repulsive chemical species of a polymer chain for additives can lead to higher water inhibition. The ability to control water permeability into the membrane by polymer design can be exploited for applications in water separation technology.

*Corresponding author
*Email addresses:* yusukearaki0109@gmail.com (Yusuke Araki), kobayashiyusei@gmail.com (Yusei Kobayashi), tohru_kawaguchi@denso.co.jp (Touru Kawaguchi), takashi_kaneko@denso.co.jp (Takashi Kaneko), arai@mech.kindai.ac.jp (Noriyoshi Arai)