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www.elsevier.com/locate/memsci

PII: S0376-7388(18)30439-3
DOI: https://doi.org/10.1016/j.memsci.2018.06.031
Reference: MEMSCI16248

To appear in: *Journal of Membrane Science*

Received date: 13 February 2018
Revised date: 4 June 2018
Accepted date: 16 June 2018

Cite this article as: Abhijit Gogoi, Tukhar Jyoti Konch, Kalyan Raidongia and K. Anki Reddy, Water and salt dynamics in multilayer graphene oxide (GO) membrane: role of lateral sheet dimensions, *Journal of Membrane Science,* https://doi.org/10.1016/j.memsci.2018.06.031

Water and salt dynamics in multilayer graphene oxide (GO) membrane: role of lateral sheet dimensions

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ABSTRACT

Dependence of salt rejection efficiency and water permeability of layered graphene oxide (GO) membranes on the lateral dimension of constituting sheets are studied through equilibrium molecular dynamic (MD) simulation and experiments. This study suggests that with increasing sheets dimension permeability of the GO membranes decreases but its selectivity increases. The velocity and permeation time of the water molecules while permeating through the membrane are influenced to a greater extent by the pore offset distance (**W**) of the membranes. More over the larger pore offset distance increases the path length that the water molecules and ions have to traverse for permeating through the layered GO membranes. Based on the simple technique discussed in this work, one can construct GO membranes of required water permeability and salt rejection without the application of any foreign nanomaterials with the GO membrane, which retains the inherent selectivity of the GO membranes. This work also provides the effect of internal structure of GO membrane on the atomistic level details of the solvation shell of ions while they are permeating through the membrane.

Keywords: Multilayer GO membrane, water permeability, salt rejection, molecular dynamics simulation, pore offset distance.

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