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Water desalination with a single-layer MoS_2 nano pore

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Recent studies in advance-nano materials has led to development of various NANO-POROUS membranes for water purification (Figure 1). By performing molecular dynamics simulation that a single layer MoS_2 (molybdenum di sulphide layer of thickness 1nm) can effectively reject salts, various ions upto 90%, provided the pore area is 20-60 A^2.These are clearly explained by permeation coefficient, energy barrier, water density, velocity distribution. For the sake of simplicity they are not discussed here.

Pores (holes through MoS_2 sheets) of range 1-10 nm were created successfully by highly focused electron beam using TEM. There is a concern about manufacturing of defect free membranes with large area. Waduge et al. have reported that a large-area, well-sealed membrane with nano pores as tiny as 2.8 nm can be fabricated. With few more efforts we can make 50Å range pores in near future.

Discussions revolve between rejection of ions & permeation of flux. Pore shape should be nozzle like structure of protein channel, as the Mo(molybdenum) atoms are hydrophilic, they attract water S(sulphur) on the other hand are hydrophobic to water and other ions. Its this combination of hydrophilic and hydrophobic centres at pore accounts for faster permeability rate than any other known material (including 70% greater than graphene). As the pore area is less rejection of ions is more. Pore area 20Å (highly hypothetical) can reject 100% of ions regard less of material chosen, but the rate of permeation will be very slow (which is a serious disadvantage). The ideal size for good permeability rate would be 40-60Å.

When water approaches S atom it slips(by repulsive force) and gets attracted to Mo atoms with more velocity and again slips at other end of sulphur atoms with even more velocity, thus crossing the pore at great speed outmatching the graphene porous membrane. It has a tensile strength about 200 GPa, comparable to steel and stable against 10 Mpa pressure in industries.

Reference

1. Mohammad Heiranian1, Amir Barati Farimani1 & Narayana R. Aluru1, a journal by nature publications

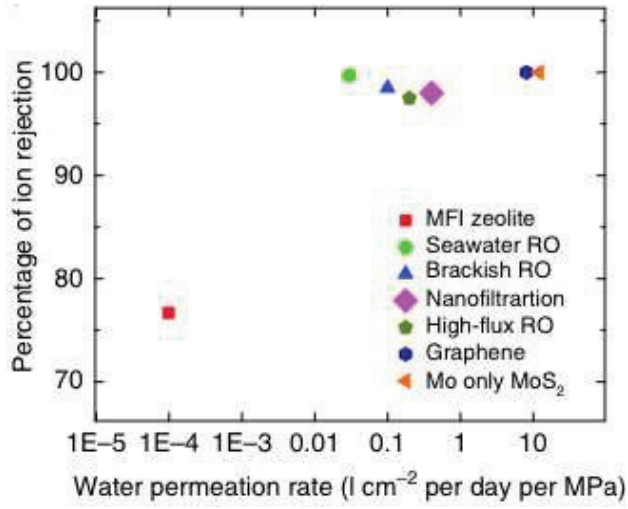

Figure 1: Comparison of various NANO-POROUS membranes for water purification