Kunalan, S.; Dey, K.; Roy, P. K.; Velachi, V.; Maiti, P. K. Palanivelu, K.; Jayaraman, N., 2020, "Efficient facilitated transport PETIM dendrimer-PVA-PEG/PTFE composite flat-bed membranes for selective removal of CO2", *J. Membr. Sci. 622*, 119007.

Collaborative work with Prof. K. Palanivelu, Anna University, Chennai and Prof. P. K. Maiti, Physics Department, IISc.

Development of membranes that provide high permeance and selectivity for separation of CO_2 gas is important in efforts towards mitigating CO_2 emission in major industrial emissions such as flue gas. Effective CO_2 capture continues to be challenging, due to issues such as stabilities and optimal performances. An avenue to increase the permeance and selectivity is through modification of membranes with CO_2-philic chelants. We herein describe high affinity dendrimer-based chelants that functionalize a cross-linked polymer membrane system. The chosen dendrimer series is the poly(propyl ether imine) (PETIM) dendrimers. These dendrimers are hither-to un-known new series to the studies of membrane functionalizations and studies. Dendrimer generations provide an advantage in order to facilitate a graded extent of the number of chelant sites within the molecule. Glutaraldehyde cross-linked poly(vinyl alcohol)–poly(ethylene glycol) membranes are functionalized further with dendrimer generations. The functionalized membranes are subjected to studies in order to adjudge CO_2 permeance and CO_2/N_2 gas mixture separation efficiencies. The functionalized dendrimers show a graded permeance and selectivity and the third generation dendrimer-functionalized membrane shows the most optimal permeance and selectivity. When adjudged through Robeson upper boundary limits, the permeance and selectivity reaches the boundary very closely, much superior to the performance of several flat-bed membranes known currently. A number of experimental variations are implemented in order to assess the dendrimer-functionalized membrane efficiencies and the stability. The experimental studies are complemented further through systematic molecular dynamic simulations. A molecular level characterization and the mechanism of CO_2 permeance and selectivity, enabled by dendrimer functionalization of the polymer membranes, are assessed. The novelty presented herein expands the scope of membranes for CO_2 separations by using a new dendrimer series that possess graded levels of high affinity CO_2 chelant sites, namely, ether imines.