

## Supplementary Information

# LadderGen: A Large-Scale Generative Library of Ladder Polymers for Membrane Separations

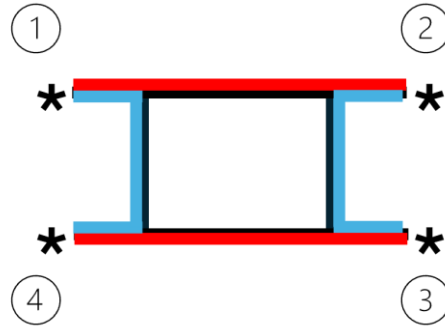
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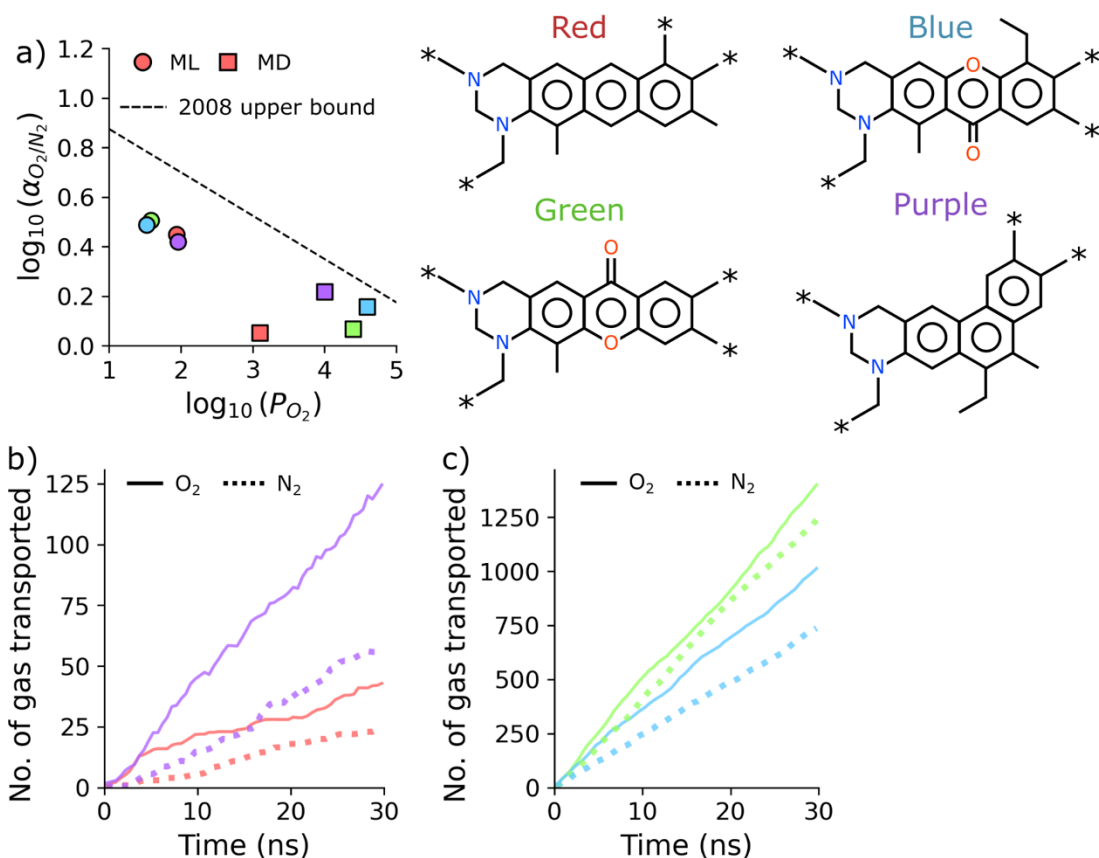
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**Fig S1. Criterion for Ladder Polymer Recognition:** Both pairings of attachment points must admit two internally vertex-disjoint paths. Specifically, for the first pairing (1 & 2 and 3 & 4), the connections are established by two non-overlapping red paths. For the second pairing (1 & 4 and 2 & 3), the connections are established by two non-overlapping blue paths.



**Fig S2. Molecular dynamics simulations for validation of negative cases.** Four polymer membranes are generated that the surrogate ML model predicts would have performance below the 2008 upper bound. (a) Predicted  $O_2/N_2$  permeability–selectivity landscape from the ML and MD. MD permeability predictions are higher than ML ones, but remain below the upper bound, as expected. (b) and (c) show the number of transported gases across the polymeric membrane.