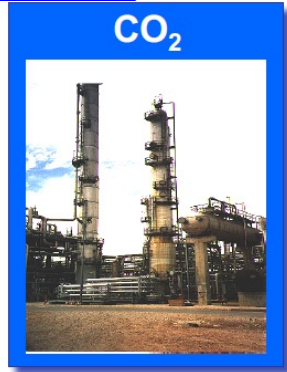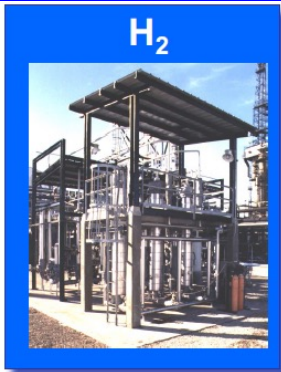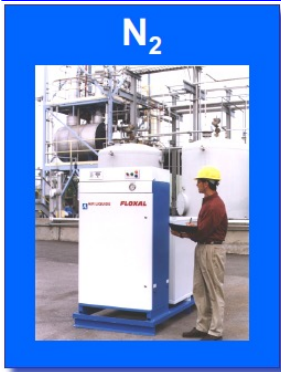# Sustainability through Materials Design

Sanat Kumar

Department of Chemical Engineering, Columbia University

Brookhaven National Laboratory, Upton, NY

Gas Separation Membranes

N₂

H₂

CO₂

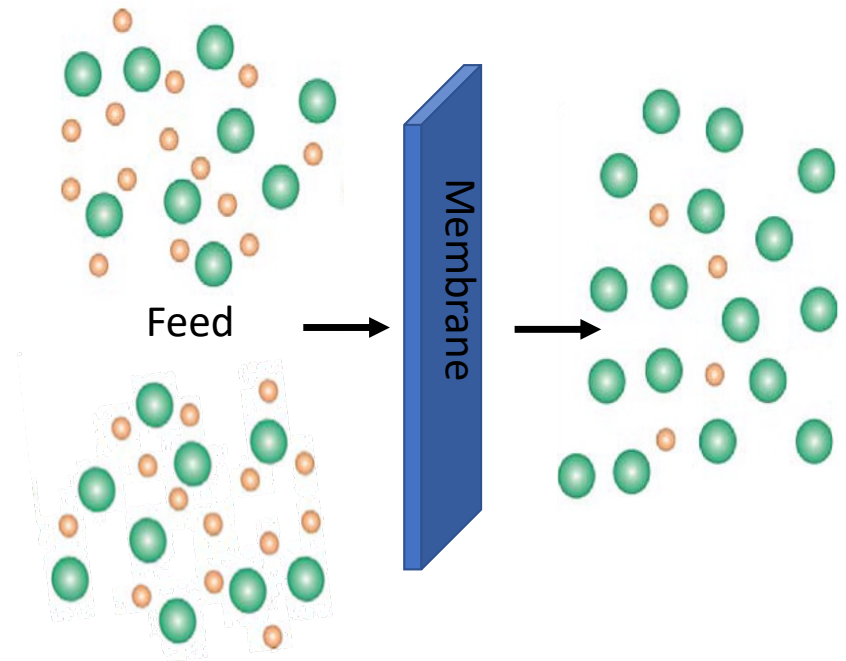Feed → Membrane →

$$|J| = D\frac{dc}{dx} = DS\frac{(\Delta p)}{\delta}$$

Diffusion
Coefficient

Solubility

Permeability
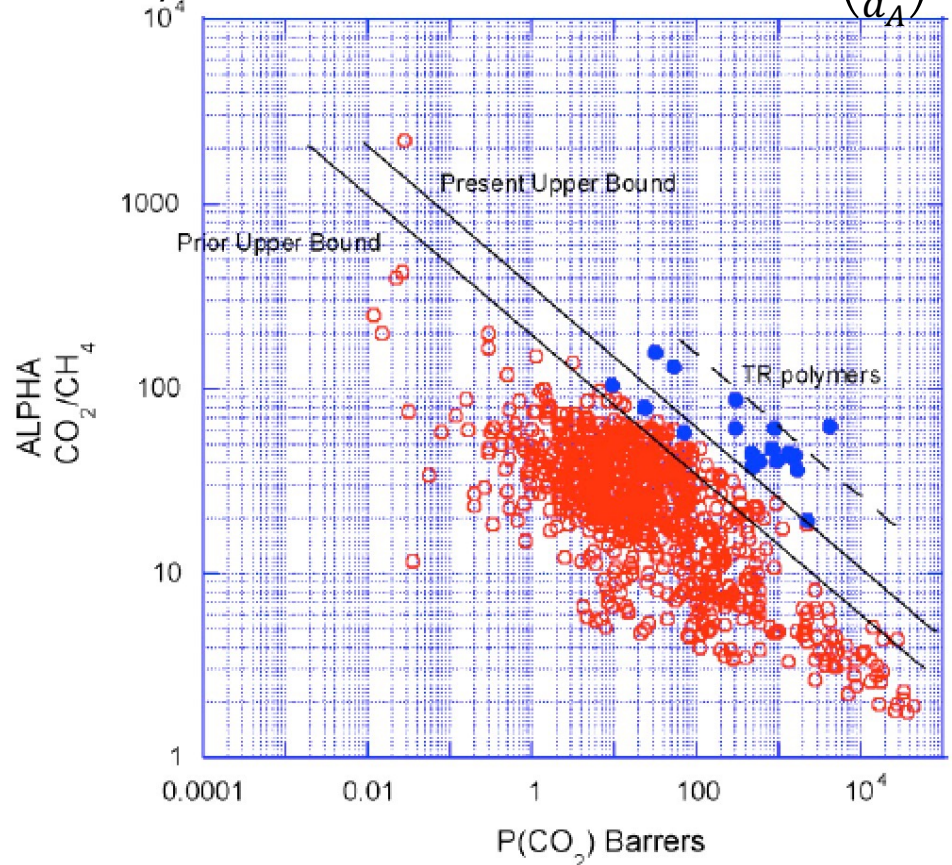
$$P_i = D_i \times S_i$$

Ideal Selectivity

$$\alpha_{i,j} = \frac{P_i}{P_j} = \frac{D_i}{D_j} \times \frac{S_i}{S_j}$$

Sieving: Robeson Upper Bound

$$ln\alpha_{A/B} = -\lambda lnP_A + \kappa \qquad \lambda = \left(\frac{d_B}{d_A}\right)^2 - 1$$

**Precious Data
(vs. Big Data)**

Robeson, J Mem Sci, 2008

Machine Learning

$$C(\mathbf{w}) = \frac{1}{2} \sum_i (y_i - \mathbf{w}^T \mathbf{x}_i)^2$$

Chemical finger print space
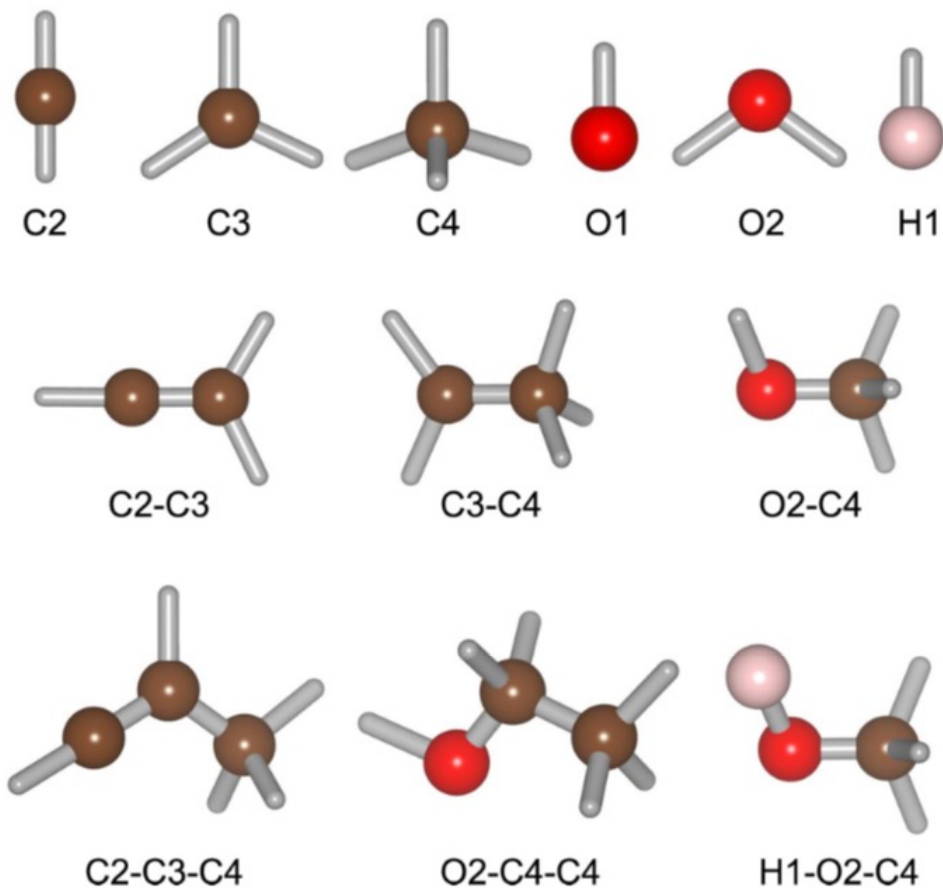
Permeability

Regularization

$$C = \frac{1}{2} \sum_i (y_i - \mathbf{w}^T \mathbf{x}_i)^2 + \frac{1}{2} \lambda ||\mathbf{w}||^2$$

Solve for λ using $\sum y_i = \sum w^T x_i$
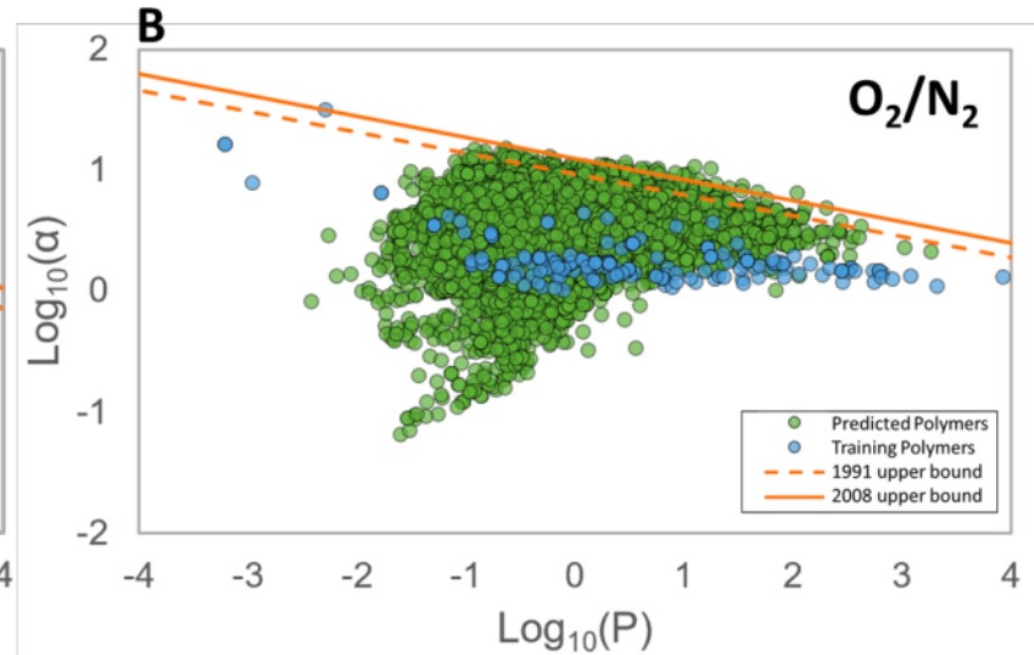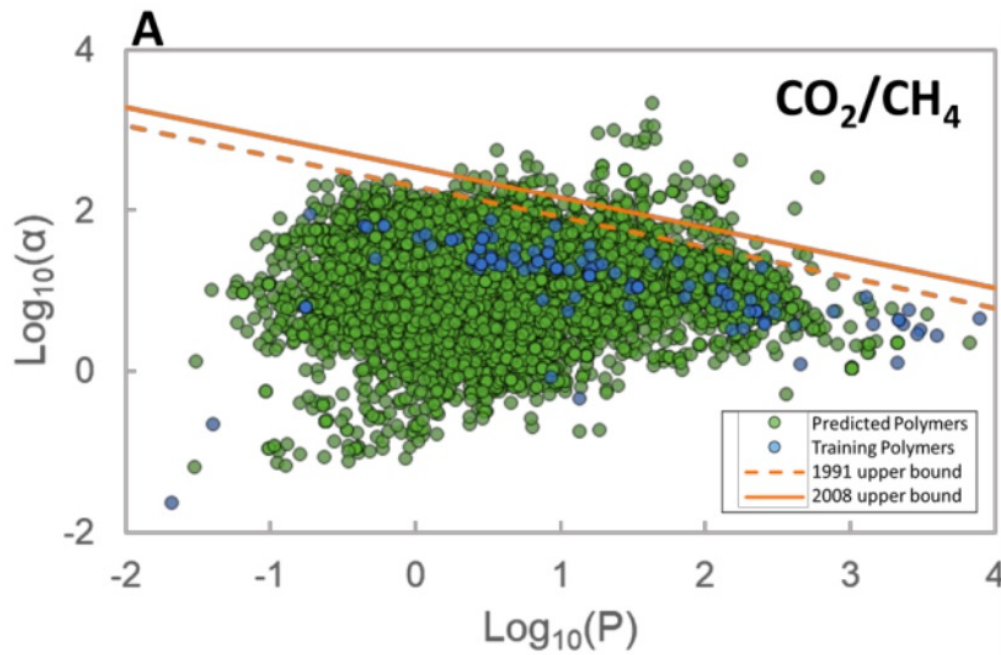**Importance of training vs test sets**

Machine Learning - Fingerprinting

C2   C3   C4   O1   O2   H1

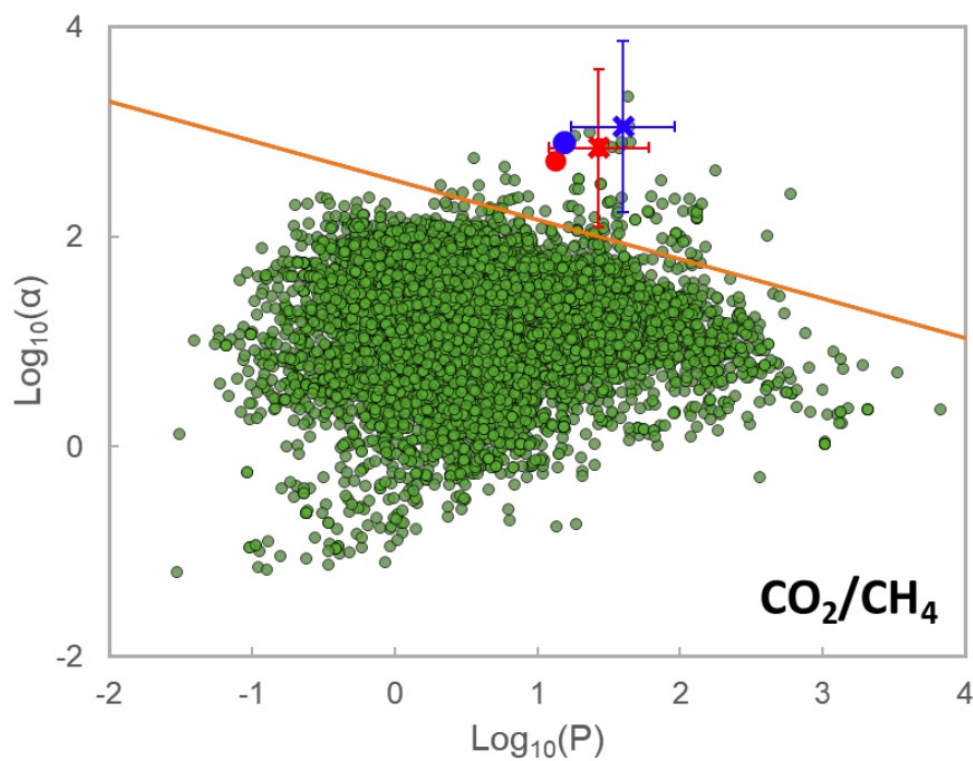C2-C3   C3-C4   O2-C4

C2-C3-C4   O2-C4-C4   H1-O2-C4

These are some of the structures and how they are modeled.

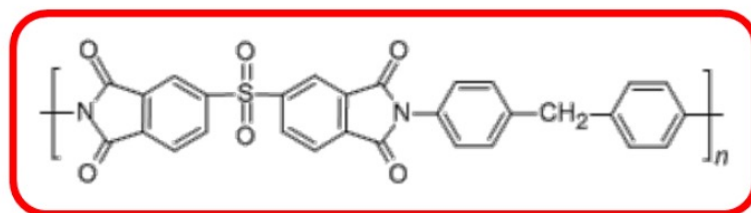# Robeson Upper Bound – MACHINE LEARNING

Robeson Upper Bound – MACHINE LEARNING

P432095

P432092
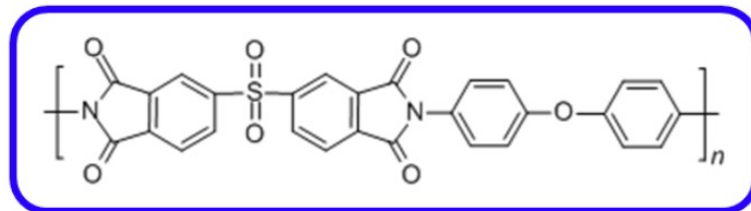
Polyimide Sulfone   Ether

CO_2/CH_4

$Log_{10}(\alpha)$

$Log_{10}(P)$

Robeson Upper Bound – MACHINE LEARNING

Machine Learning is going to play a central role.

Molecular Structure is important. Use of ML alone is not enough.

Molecular Modeling and Experiments are important