Efficient Nanopore Optimization by CNN-accelerated Deep Reinforcement Learning

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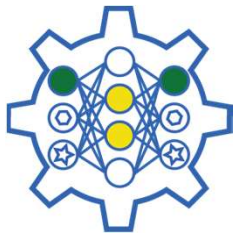
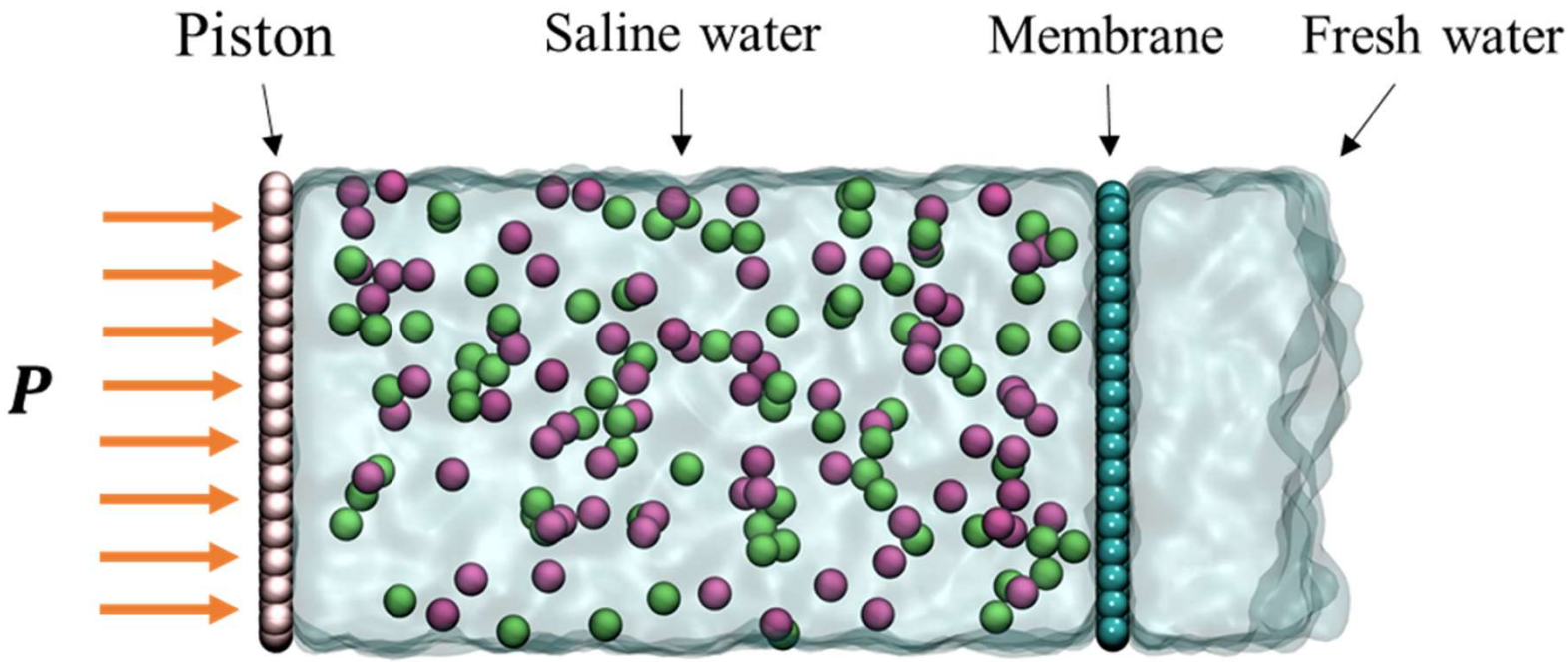
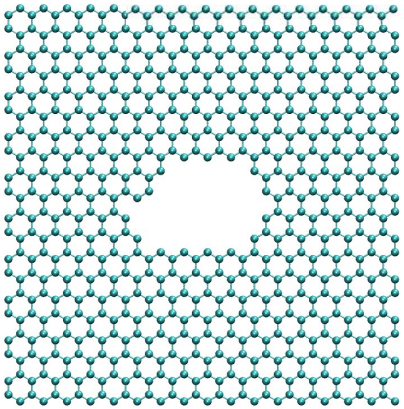


Motivation: Effect of pore geometry in water desalination

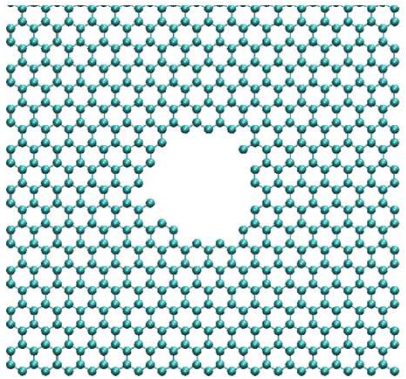




Area: ~64 Å^2

Flux: 73 molecules/ns

Ion rejection: 98.06%



Area: ~64 Å^2

Flux: 62.25 molecules/ns

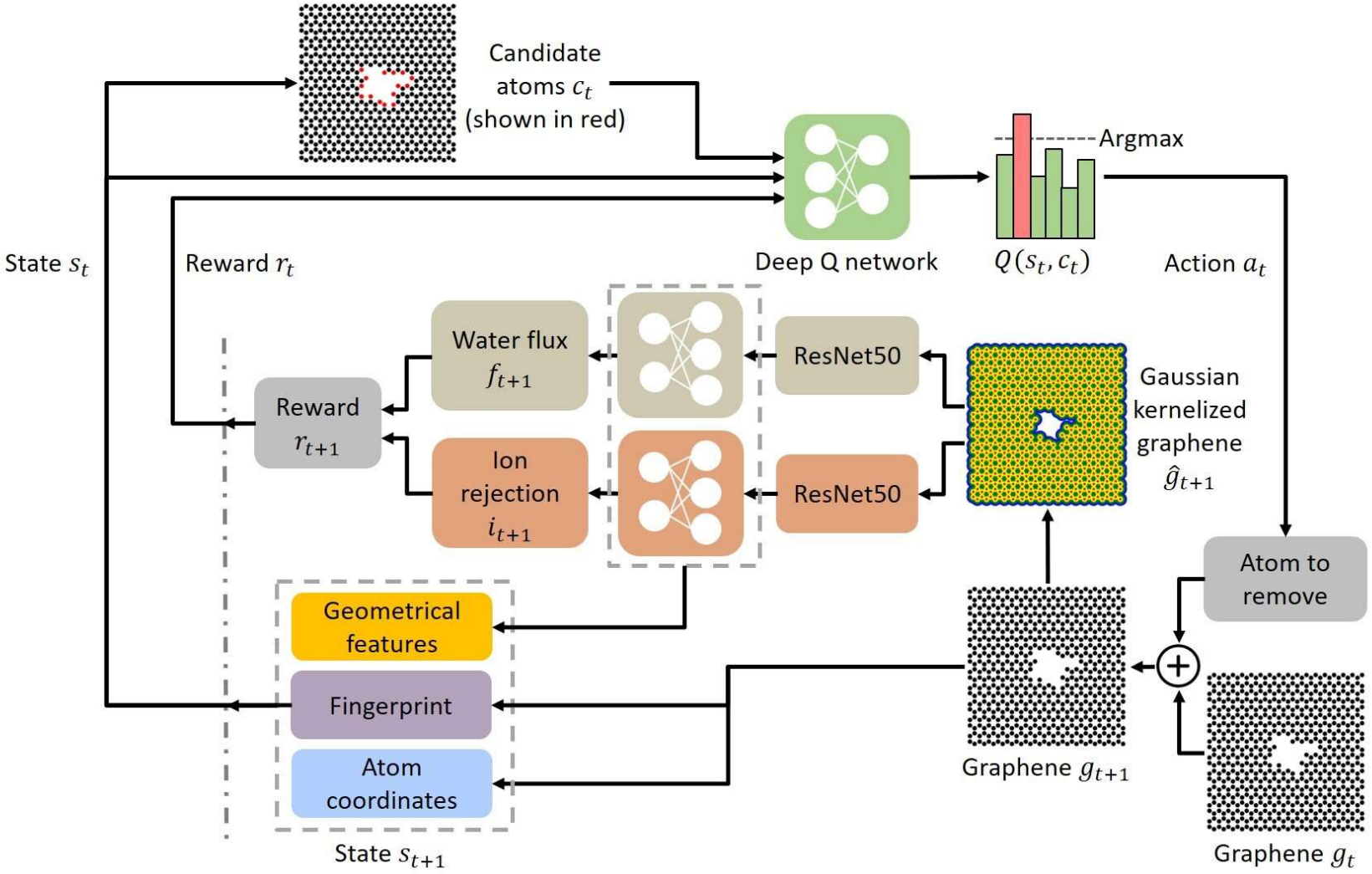
Ion rejection: 97.42%

Optimal pore: Maximize water flux while keeping high ion rejection rate

Finding the optimal pore geometry: challenges

- Millions of possible geometries
- Getting the water flux & ion rejection of a single pore requires 10 ns MD simulation (36 hours on 56-core CPU cluster). 1000 pores = ~4.1 years
- Is there any time and cost efficient method for optimizing? Yes, Deep Reinforcement Learning (**DRL**)

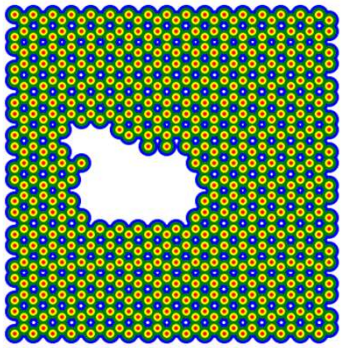
DRL Pipeline for optimizing graphene nanopores



Water desalination performance predictor:
Enables rapid reward calculation and makes DRL training possible

Water Desalination Performance Predictor

Convolutional Neural Network (CNN)



Geometrical feature
(Image format)

CNN feature extractor:
ResNet18,
ResNet50,
VGG16

Output: Vector size of 1000

MLP:
(1000, 256)
(256, 64)
(64, 1)

Water flux

or

Ion rejection

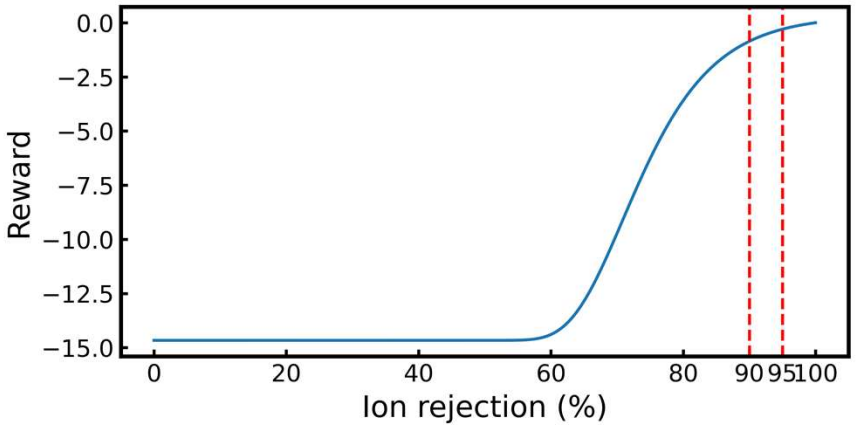
Model	Flux MSE	Flux R^2	Ion rejection MSE	Ion rejection R^2
VGG16 [24]	0.0448	0.957	0.0156	0.985
ResNet18 [25]	0.0024	0.998	0.0039	0.996
ResNet50 [25]	0.0022	0.998	0.0038	0.996

The model is trained on a dataset with 3937 samples augmented
from 185 simulation result

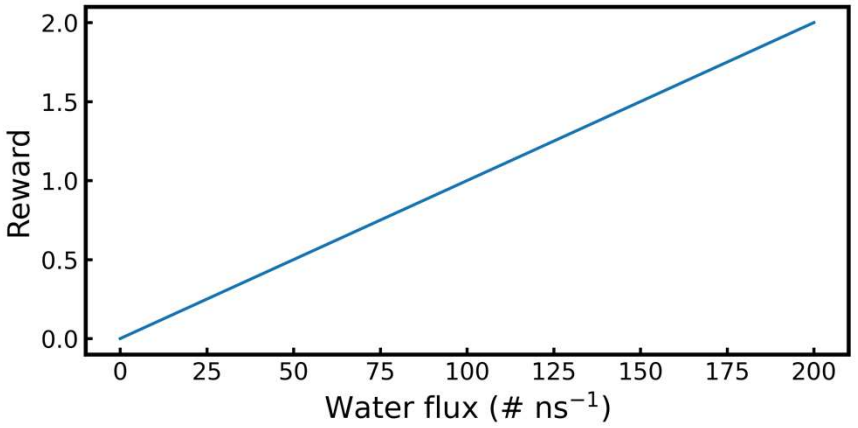
DRL: Reward function

$$\sigma(x) = A + \frac{K - A}{(C + Qe^{-Bx})^{\frac{1}{\nu}}}$$

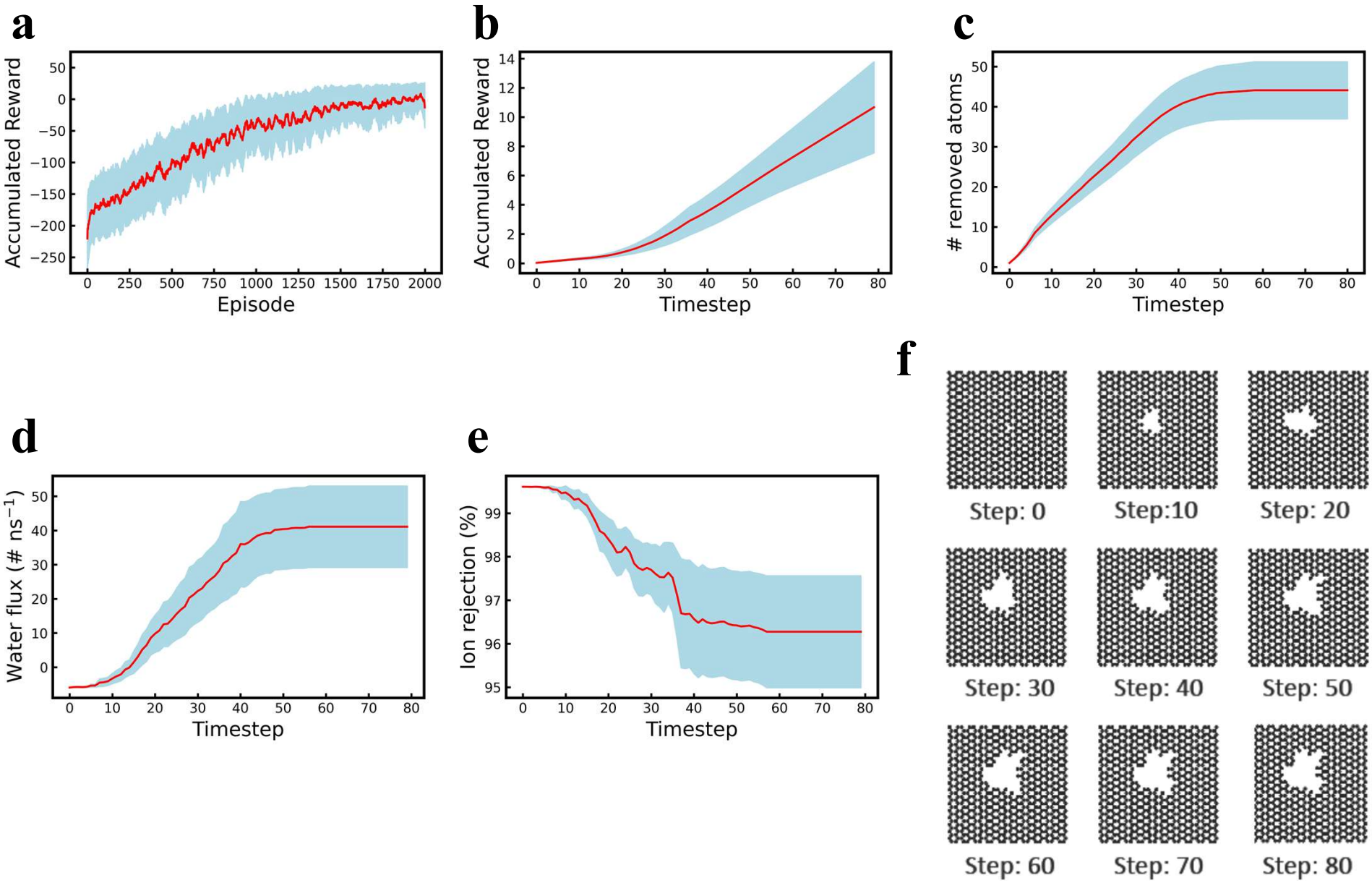
$$A = -15,\ K = 0,\ B = 13,\ Q = 100,\ \nu = 0.01,\ C = 1$$



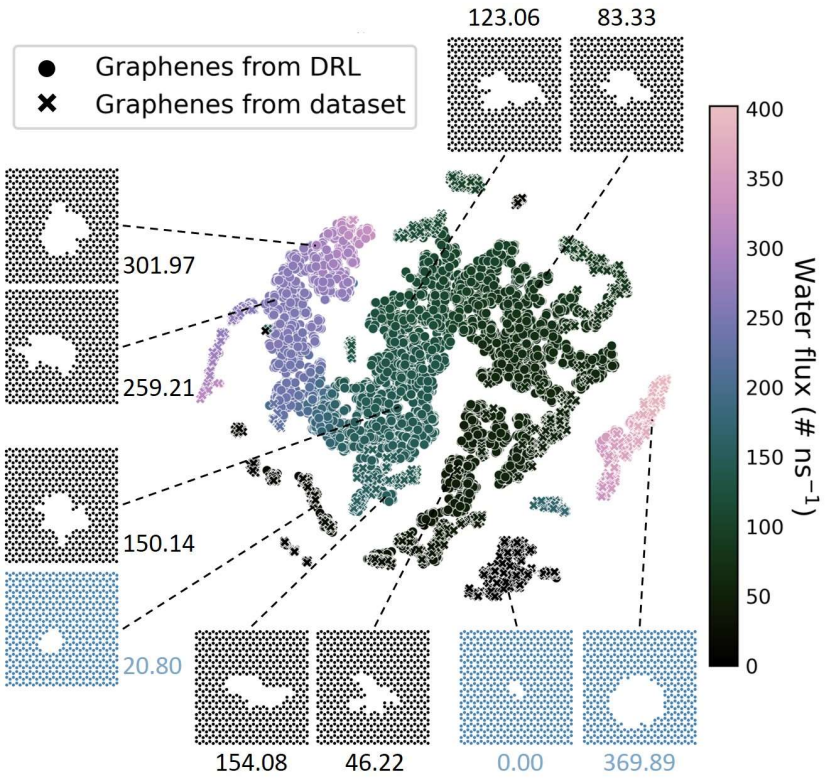
$$r_t = \alpha f_t + \sigma(i_t) - \sigma(1)$$

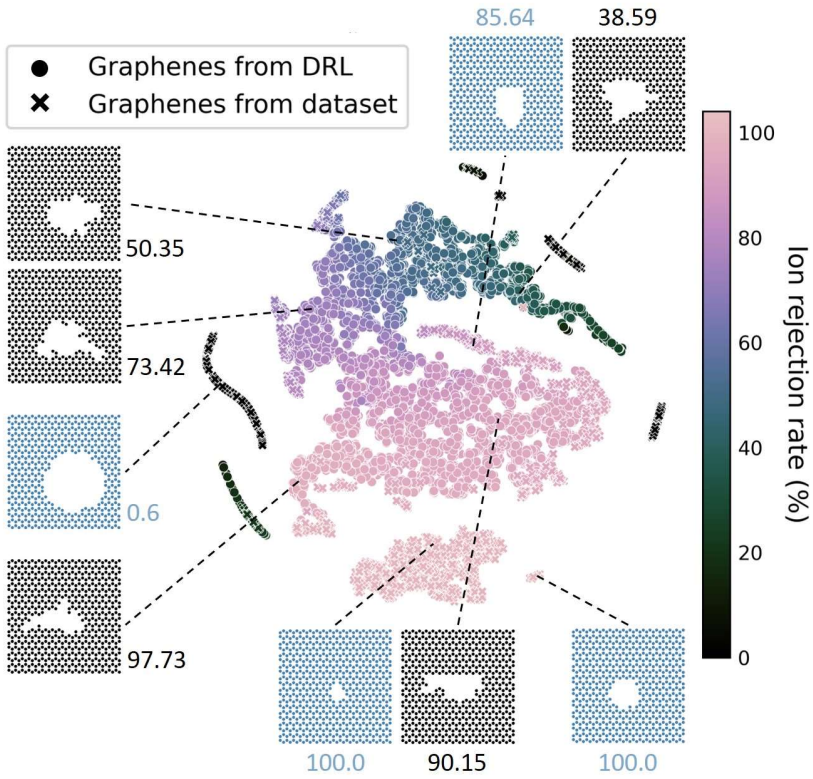


Results: DRL Training



Results: T-SNE on pores



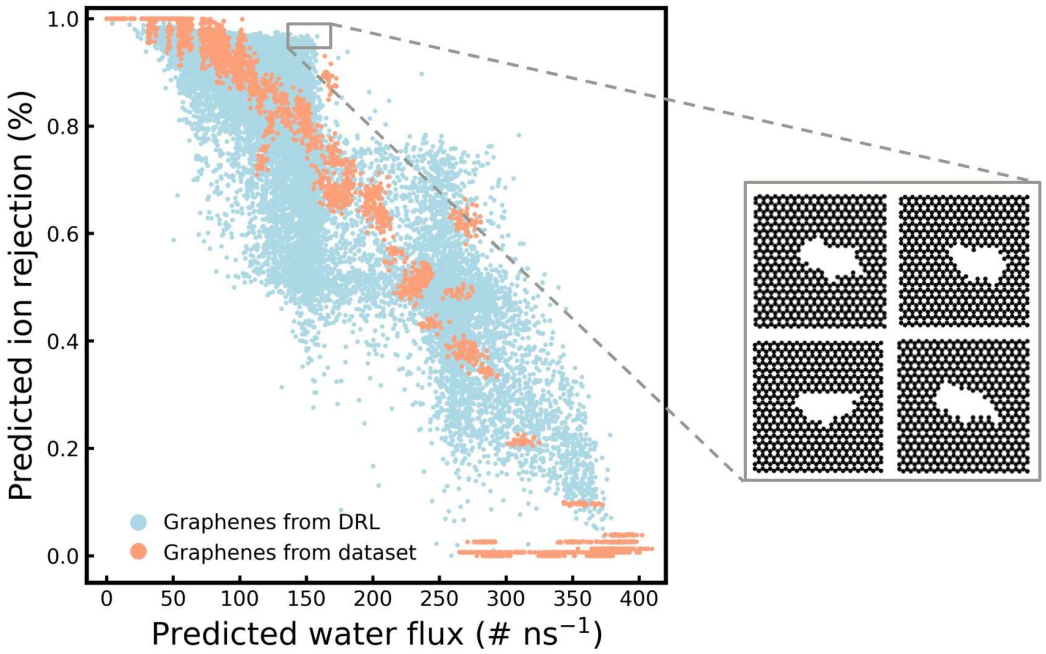


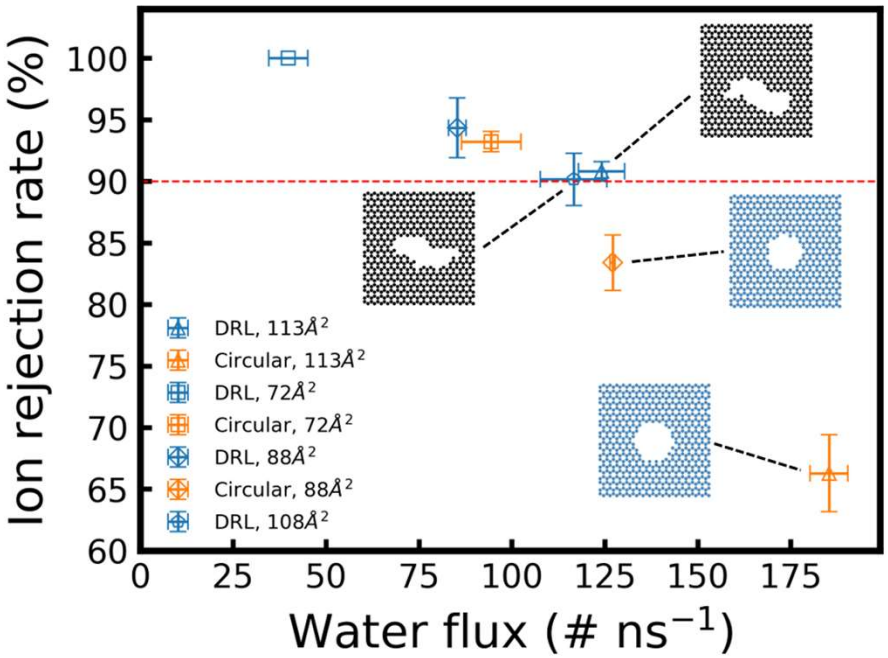
ResNet50 extracted features (1000 dimensions) => 2 dimensions

7999 DRL generated pores + 3937 training samples

Evaluating 7999 pores could take 33 years
using MD simulation on a 56-core CPU machine!

Results: How's the performance of DRL generated pores?





Questions?