Efficient Nanopore Optimization by CNN-accelerated Deep Reinforcement Learning

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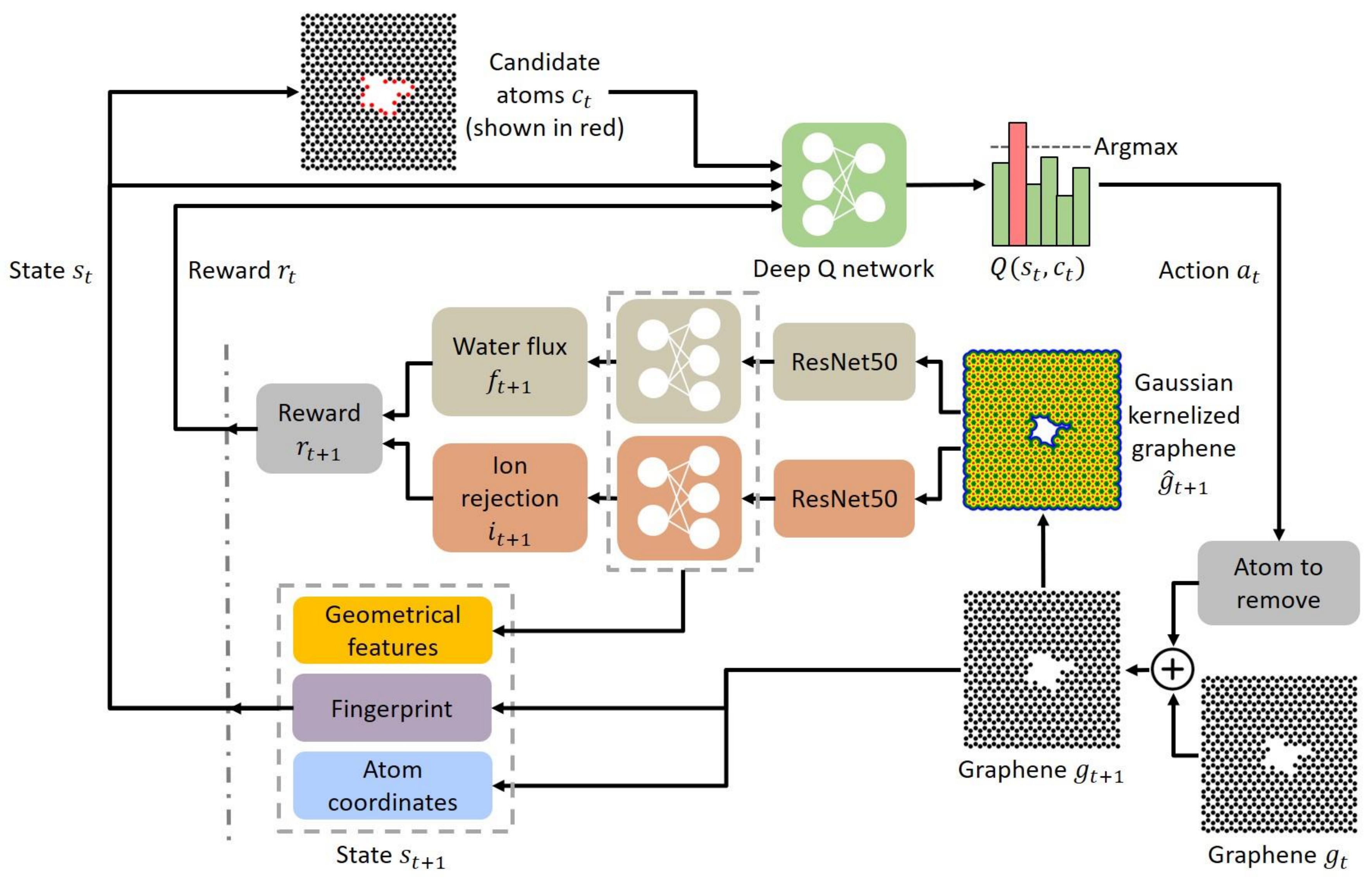
Abstract

Challenge: Structure and geometry optimization of nanopores on 2D materials is beneficial for their performance in real-world engineering applications such as water desalination [1,2]. However, the optimization process often involves very large numbers of experiments or simulations which are expensive and time-consuming.

Our work: In this work, we propose a graphene nanopore optimization framework via the combination of deep reinforcement learning (DRL) [3] and convolutional neural network (CNN) [4] for efficient water desalination. The DRL agent controls the geometry of nanopore, while the CNN is employed to predict the water flux and ion rejection of the nanoporous graphene membrane at a certain external pressure.

Method



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

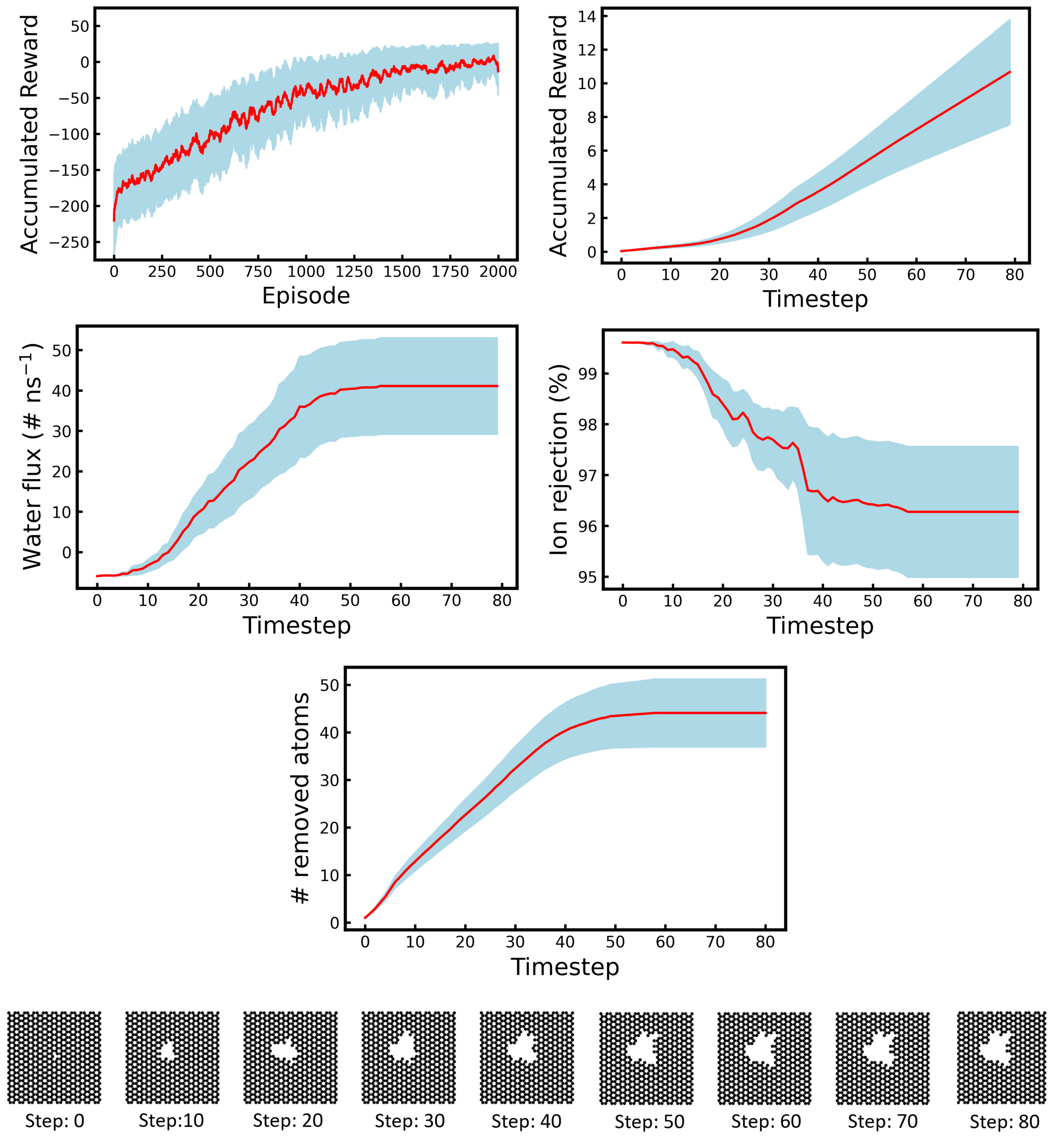
$$r_t = \alpha f_t + \sigma(i_t) - \sigma(1)$$

At each timestep, the nanoporous graphene structure is fed into a neural network to estimate water flux and ion rejection rate. Also the geometrical features extracted from the performance predictor is concatenated with the fingerprint and atom coordinates for the current state. Given the current graphene structure, candidate atoms are picked which locate at the edge of the nanopore. The RL agent constructed upon Deep Q-network takes as input the reward, candidate atoms, and state to determine the next atom to remove from the graphene.

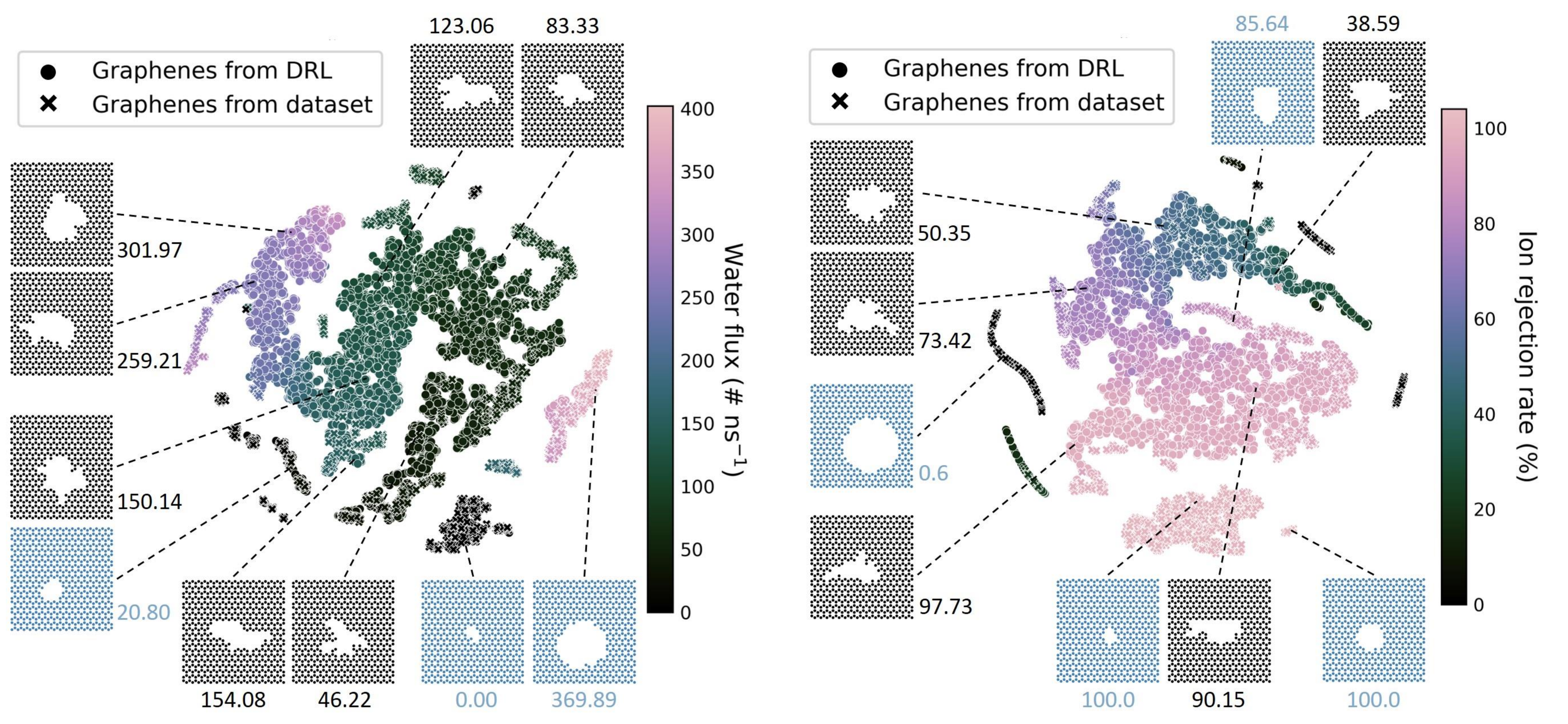
Experiment Results

Table 1: Performance of different models for graphene property prediction.

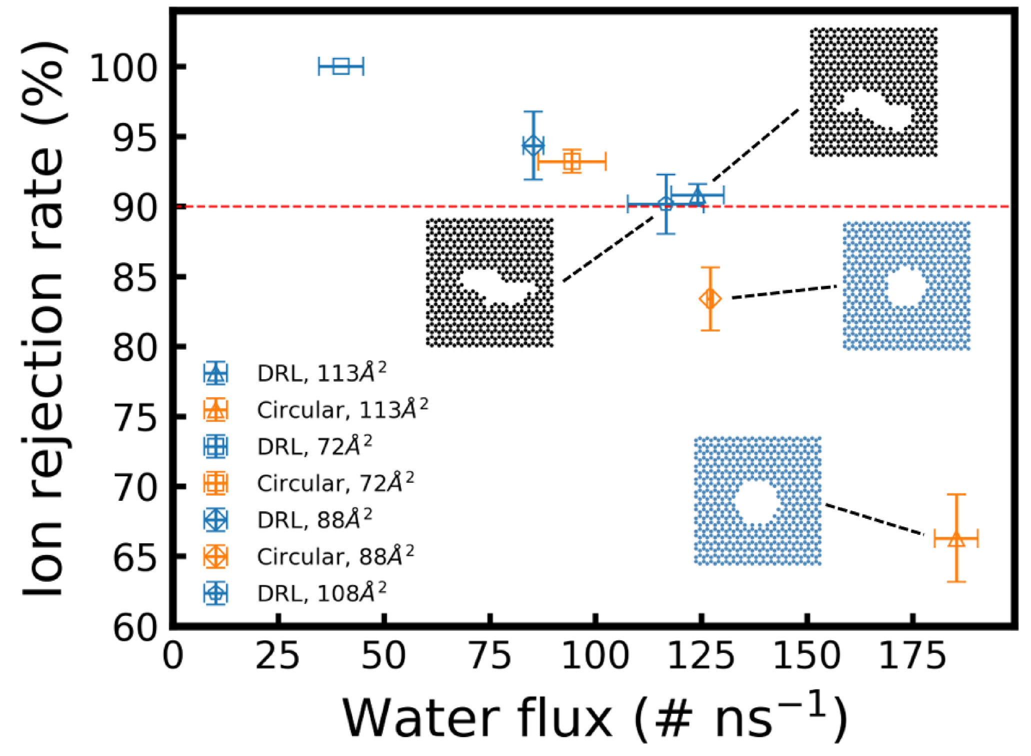
Model	Flux MSE	Flux R^2	Ion rejection MSE	Ion rejection R^2
VGG16 [24]	0.0448	0.957	0.0156	0.985
ResNet18 [25]	0.0024	0.998	0.0039	0.996
ResNet50 [25]	0.0022	0.998	0.0038	0.996



Training results for 10 DRL agents and evolution of a graphene nanopore designed by DRL agent. The DRL agent learns to control the growth of nanopore and stops after the nanopore area is large enough to allow high water flux while retains a sufficient ion rejection rate.



The collection of both DRL generated nanoporous graphene membranes (7999 samples) and mem-branes in the training dataset (3937 samples) is visualized using T-SNE. In this work, using CNN extracted features from each graphene membrane, T-SNE successfully clustered samples with similar water flux or ion rejection. This result indicates that features extracted from CNN modelshave a strong correlation with the water flux and ion rejection rate.



As shown, when the pore area is 113Å^2, DRL generated nanopore maintained over 90% ion rejection rate while the circular pore rejects only approximately 65% of ions even though allowing higher water flux. A pore with high water flux but a very low ion rejection rate is not desirable in water desalination application.

References:

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