# Deciphering Ion Specificity at Water-Mediated Graphene Interfaces via Interpretable Machine Learning

Lingzhi Cao[a], Haochen Feng[a], Jefferson Zhe Liu[a], Dan Li[b]

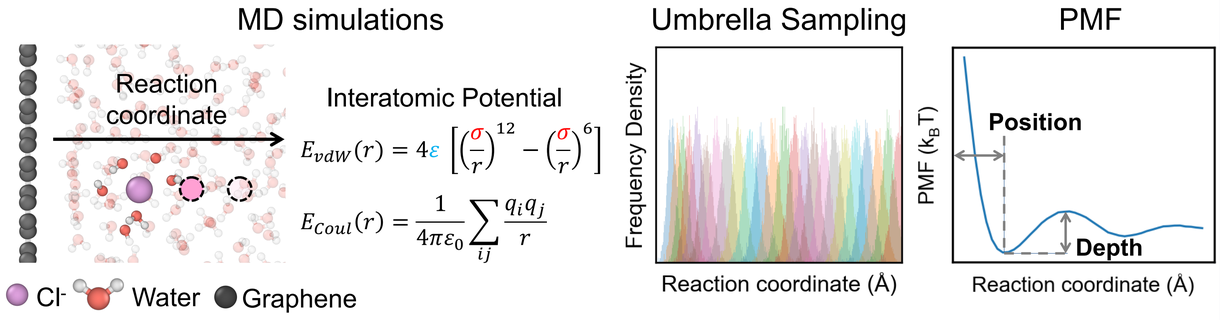
[a] The University of Melbourne, [b] The Hong Kong University of Science and Technology

## Introduction

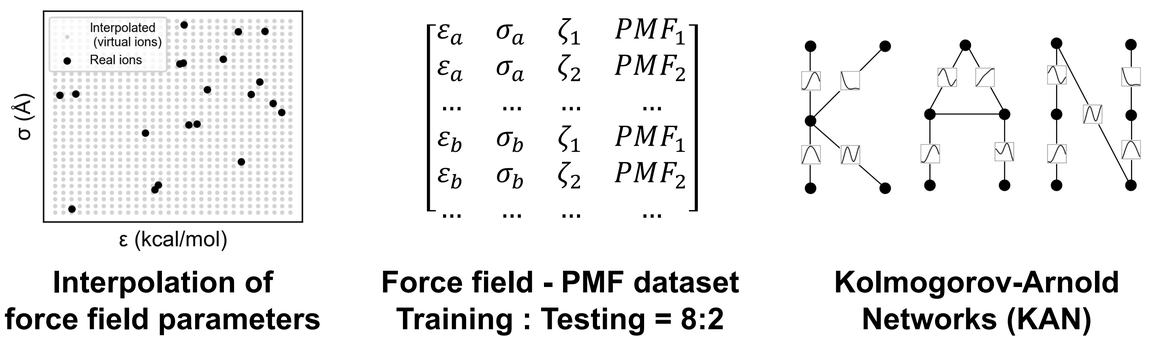
- ***Ion–surface potential of the mean forces (PMFs)*** at aqueous interfaces encode essential information for understanding adsorption and selectivity.
- Surprisingly, ***different force fields yield nearly identical PMFs*** for ions at the graphene/water interface, despite prominent differences in parameters.
- The observation motivates an exploration of how ***microscopic force field parameters*** shape PMFs under the ***influence of interfacial water***.
- This work highlights the power of AI-driven modeling in resolving ***many-body interactions at complex interfaces*** and offers interpretable insight into the physical origin of ion specificity.

## Methods

### Molecular Dynamics (MD) Simulations and Umbrella Sampling

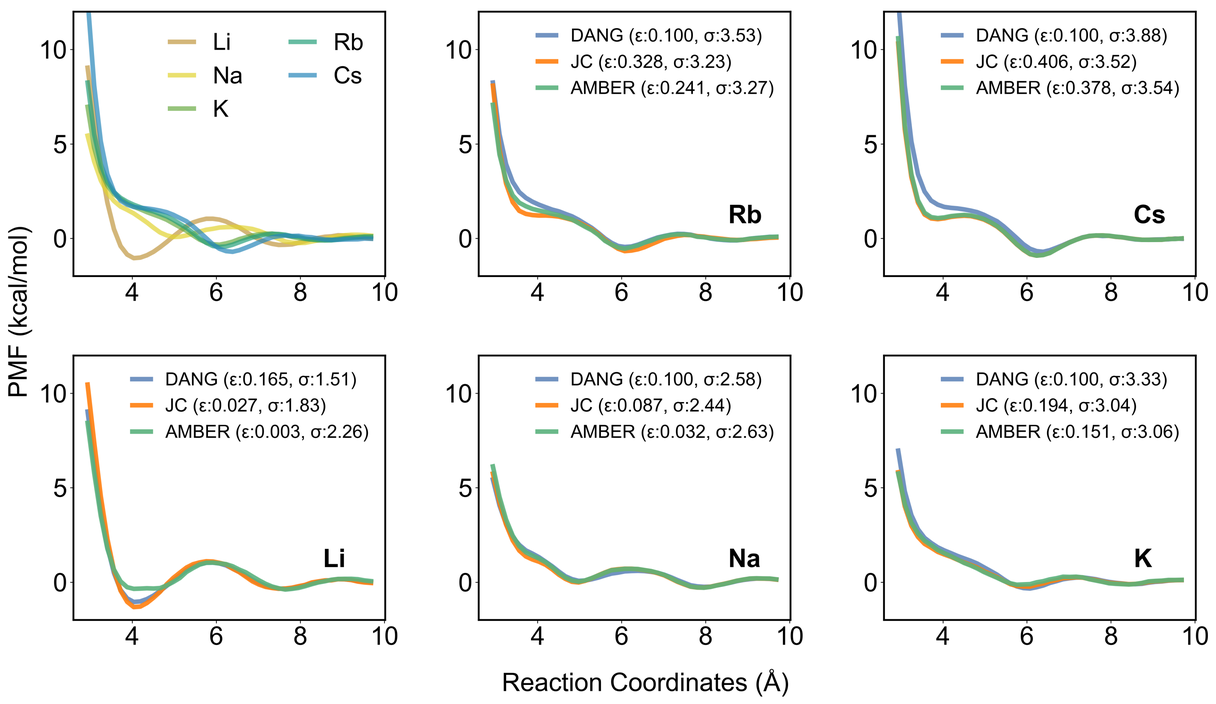



### Training Neural Networks to Learn PMF



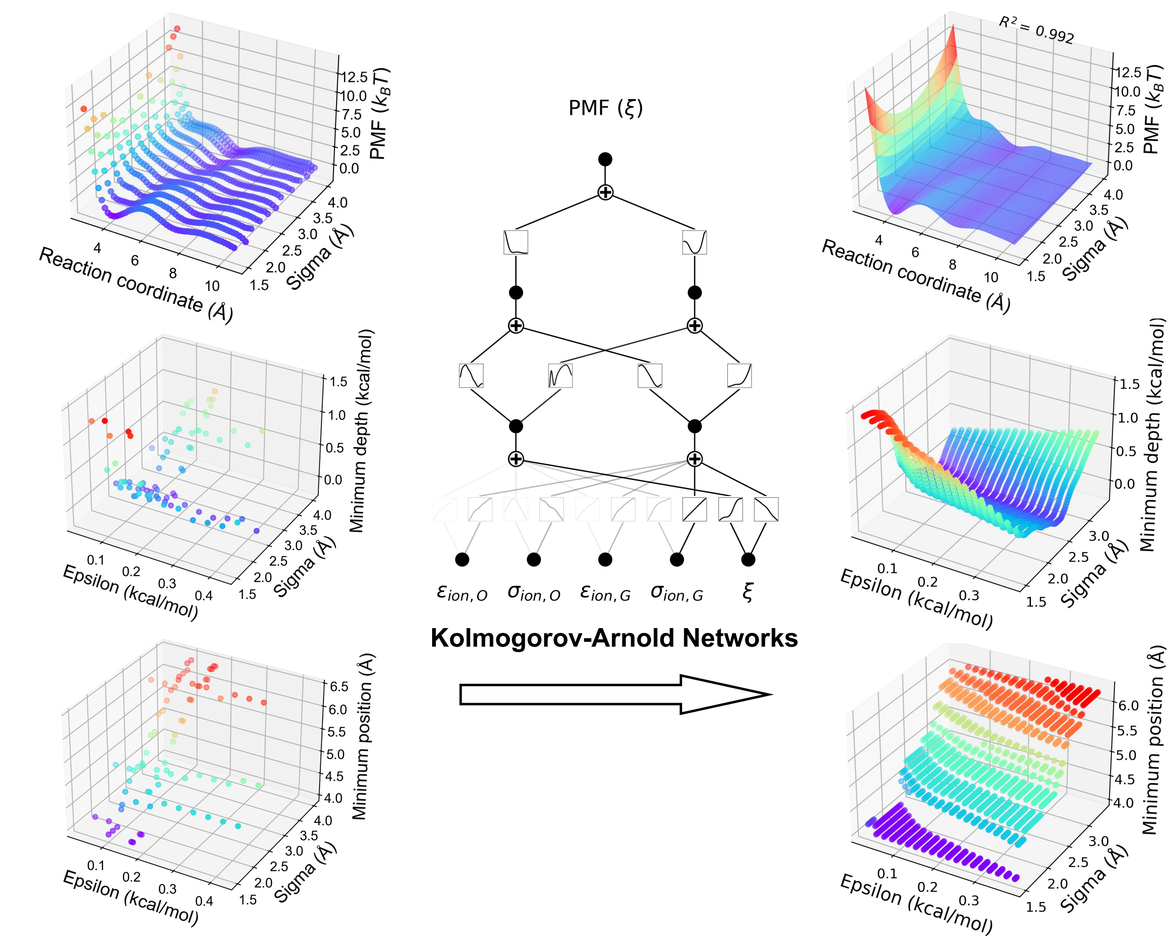

## Results and Discussion

### Emergent Ion Specificity Across Divergent Force Fields




- Nearly identical PMF curve features, yet drastically different Lennard-Jones force field parameters.

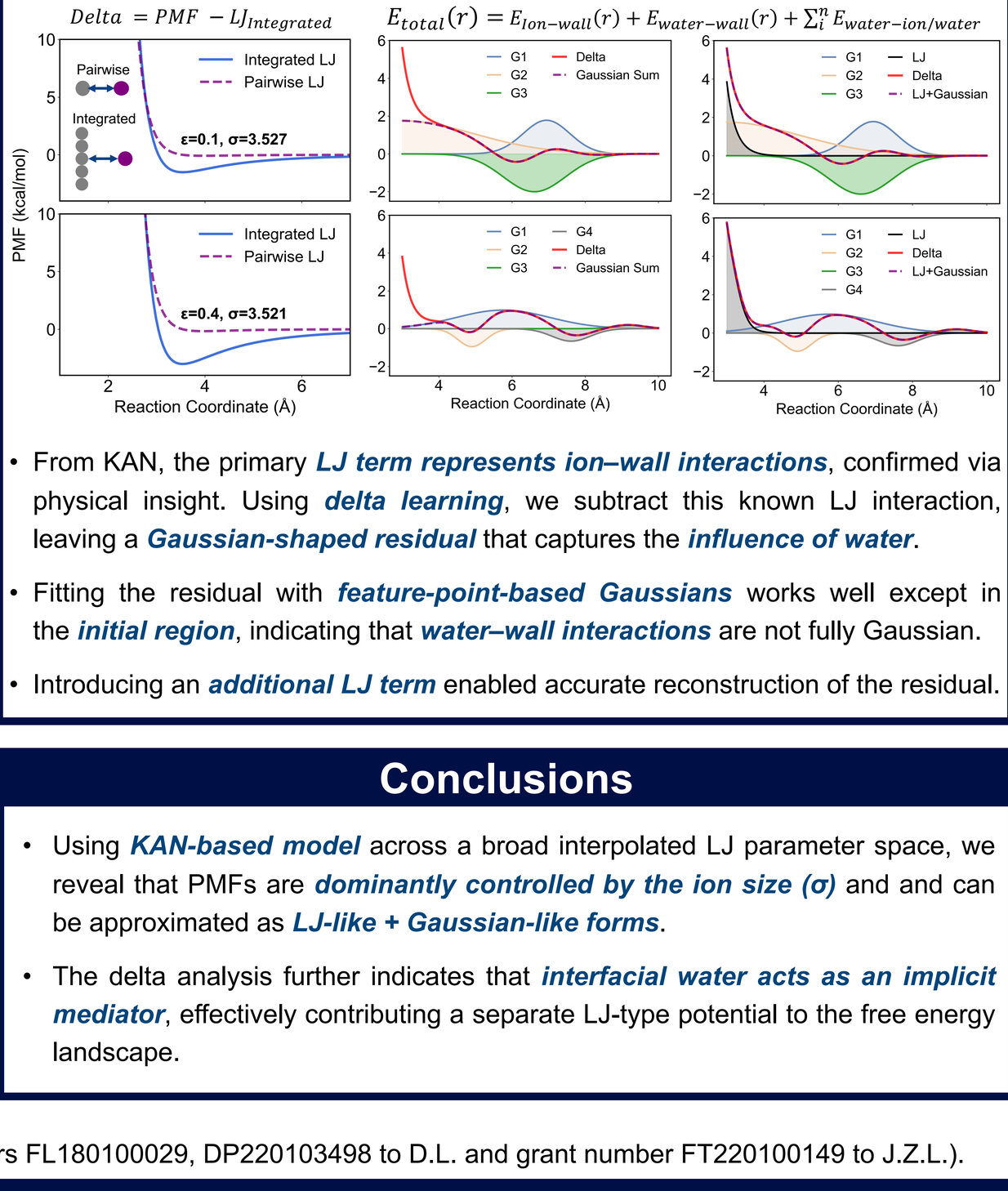
### Learning the PMF Landscape from Interpolated Force Fields




$$PMF = Gaussian_{water-ion} + LJ_{water-graphene}$$

- The KAN fitted data well, suggesting PMF is a ***Lennard-Jones + Gaussian*** form.
- The augmented data indicate ***σ has a stronger influence on PMF shape than ε***.

### Physics-Informed Decomposition of PMF




- From KAN, the primary ***LJ term represents ion–wall interactions***, confirmed via physical insight. Using ***delta learning***, we subtract this known LJ interaction, leaving a ***Gaussian-shaped residual*** that captures the ***influence of water***.
- Fitting the residual with ***feature-point-based Gaussians*** works well except in the ***initial region***, indicating that ***water–wall interactions*** are not fully Gaussian.
- Introducing an ***additional LJ term*** enabled accurate reconstruction of the residual.

## Conclusions

- Using ***KAN-based model*** across a broad interpolated LJ parameter space, we reveal that PMFs are ***dominantly controlled by the ion size (σ)*** and and can be approximated as ***LJ-like + Gaussian-like forms***.
- The delta analysis further indicates that ***interfacial water acts as an implicit mediator***, effectively contributing a separate LJ-type potential to the free energy landscape.

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zhe.liu@unimelb.edu.au
dan.li@ust.hk