

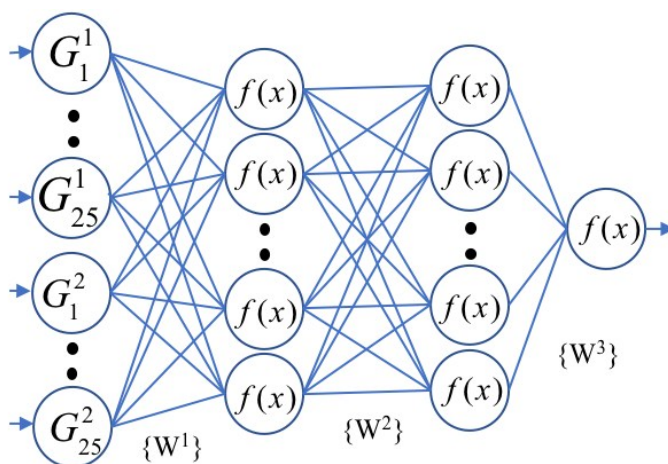
## Supporting Information

### Active Learning a Coarse-Grained Neural Network Model for Bulk Water From Sparse Training Data

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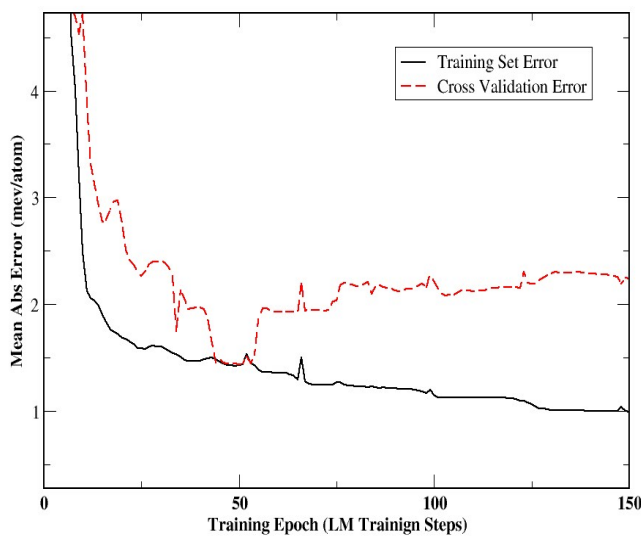
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Neural Network Architecture:



**Figure S1:** Schematic of the NN employed in this work. The network parameters used here was taken from previous work (Appl. Phys. Lett. 115, 193101 (2019)) in order to maintain an accurate comparison between this network and networks trained using more traditional approaches.

### Validation and Training Errors:



**Figure S2:** Training and validation error as a function of LM training steps during any given AL cycle. The network with the lowest validation error is chosen for the next AL cycle.