

## Supporting Information

### **Machine learning-guided investigation for a high-performance electrochromic device based on ammonium metatungstate-iron (II) chloride-heavy water electrochromic liquid**

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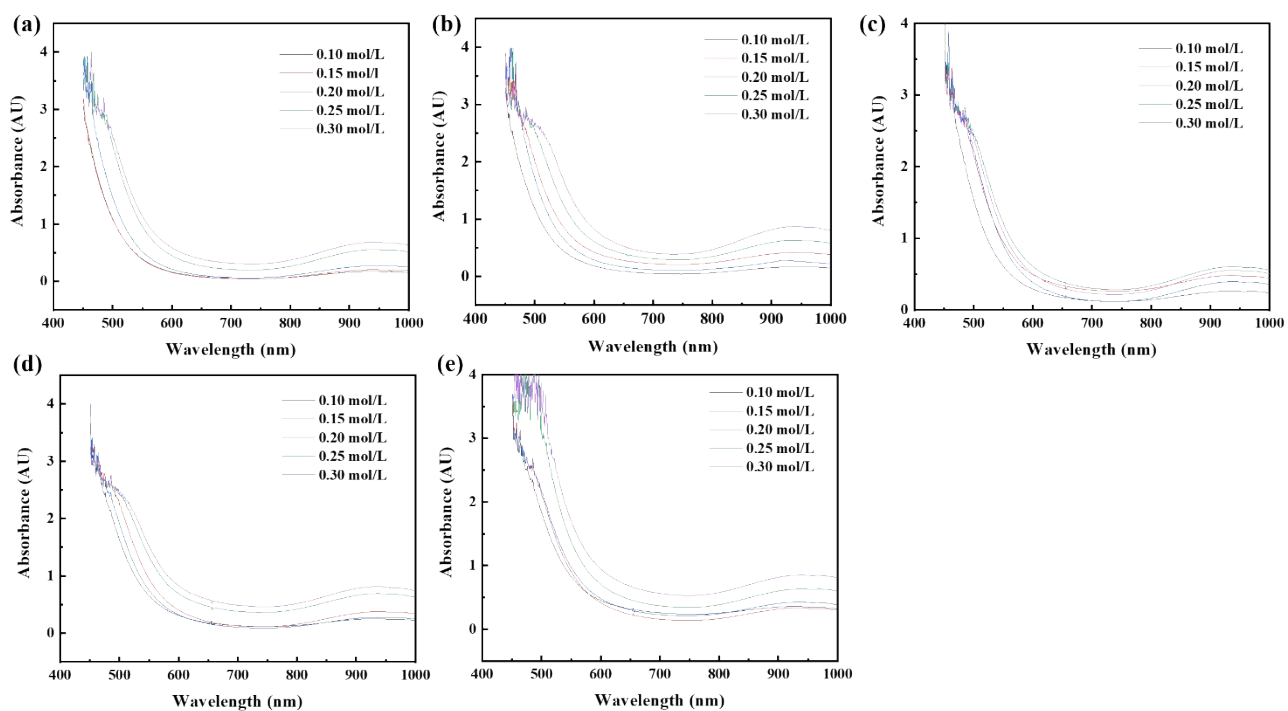


Fig. S1. Absorbance spectra of solution samples with different concentrations of ammonium metatungstate: (a) 0.100 mol/L, (b) 0.125 mol/L, (c) 0.150 mol/L, (d) 0.175 mol/L, (e) 0.200 mol/L. In each panel, the solution samples have the same concentration of ammonium metatungstate and five different concentrations of iron (II) chloride.

Figs. S1a-e show the red shift of the absorbance spectrum with increasing concentration of iron (II) chloride, confirming that the mixture of ammonium metatungstate and iron (II) chloride is successfully formed.

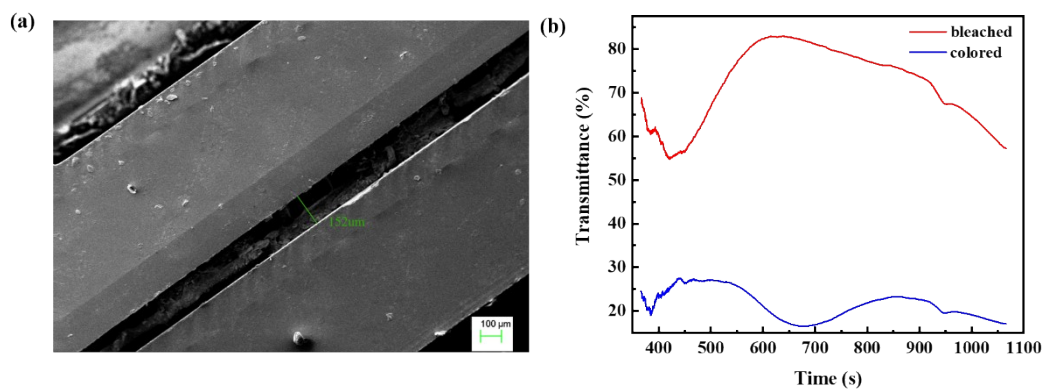


Fig. S2. (a) Confocal laser scanning microscope (CLSM) image and (b) optical transmittance spectra of a typical device.

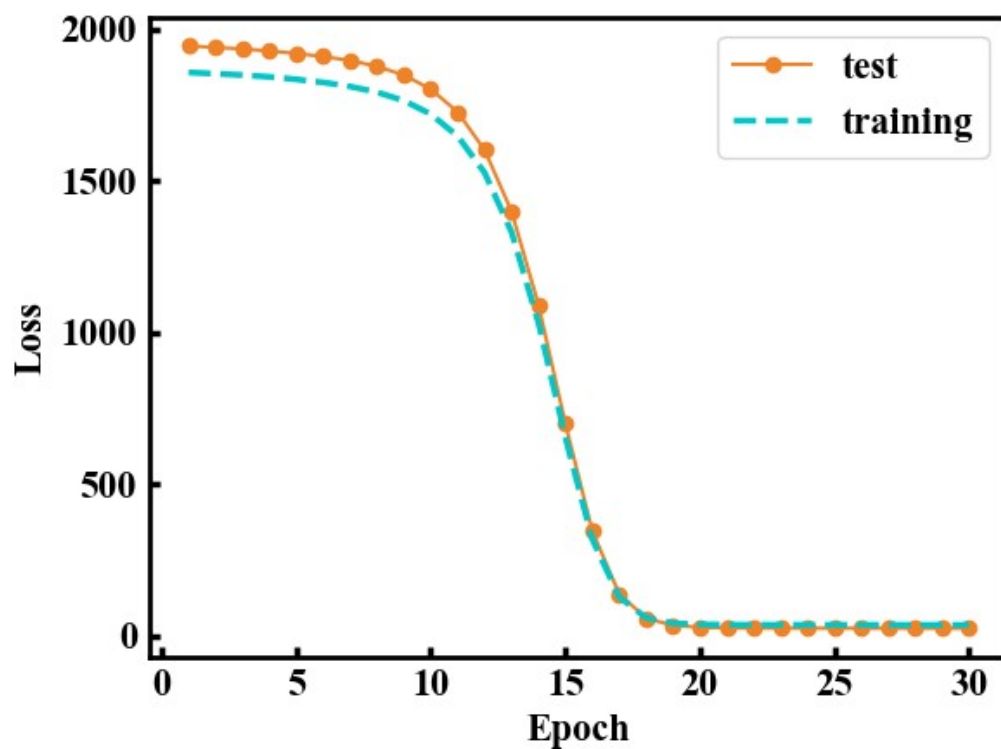


Fig. S3. Loss curves of the MLP model on the training and test sets.

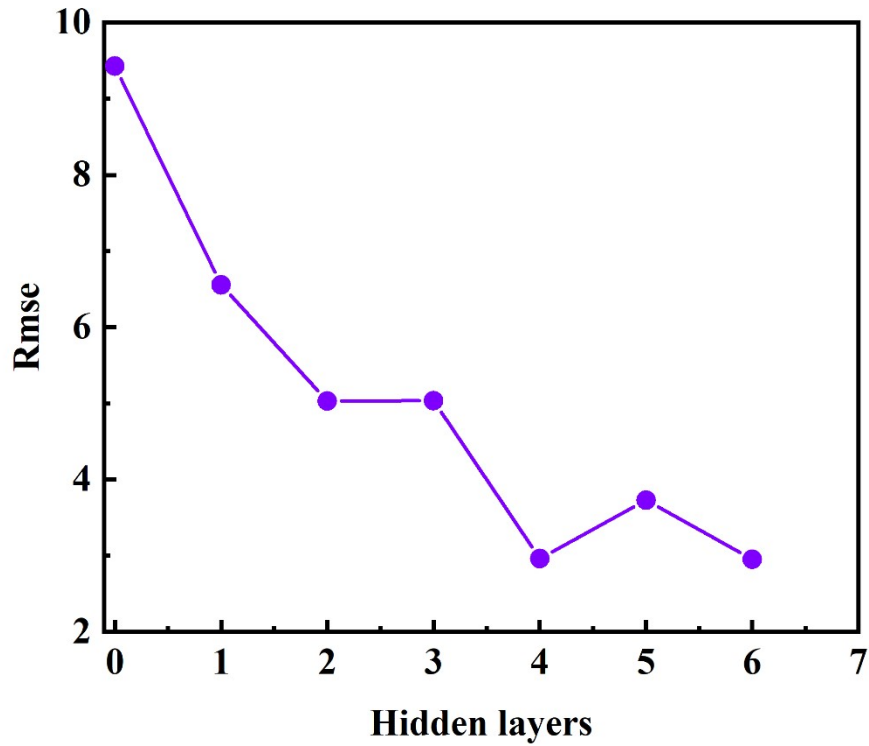


Fig. S4. (a) RMSE on the test set as a function of the number of hidden layers.

As shown in Fig. S4, RMSE continues to decrease as the number of hidden layers increases from 0 to 4, but it becomes almost saturated when the number of hidden layers exceeds 4. To achieve a sufficiently low RMSE and simultaneously keep the network structure as simple as possible, the optimal number of hidden layers has been set to 4.