Supplementary information

Crystal graph convolution neural networks for fast and accurate prediction of adsorption ability of Nb_2CT_x towards Pb(II) and Cd(II) ions

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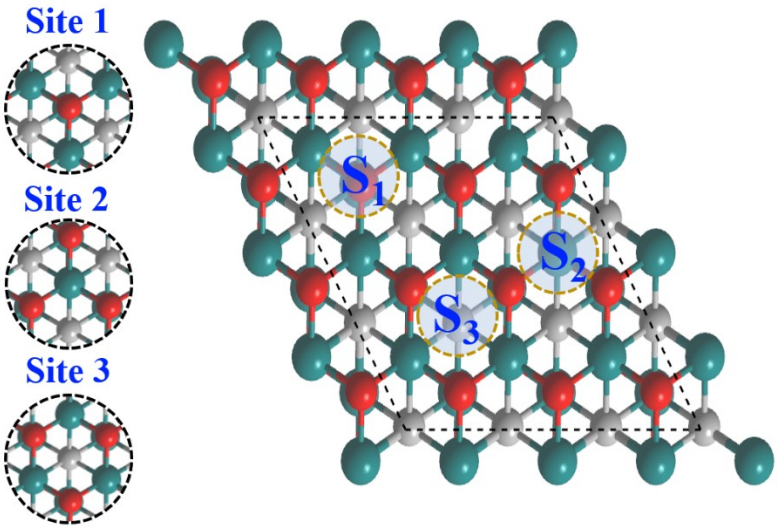

Fig. S1. Top view of the optimized crystal structure of Nb_2CT_x with 3 × 3 × 1 supercell. (S1–S3) represent the possible adsorption sites for heavy metal ions.

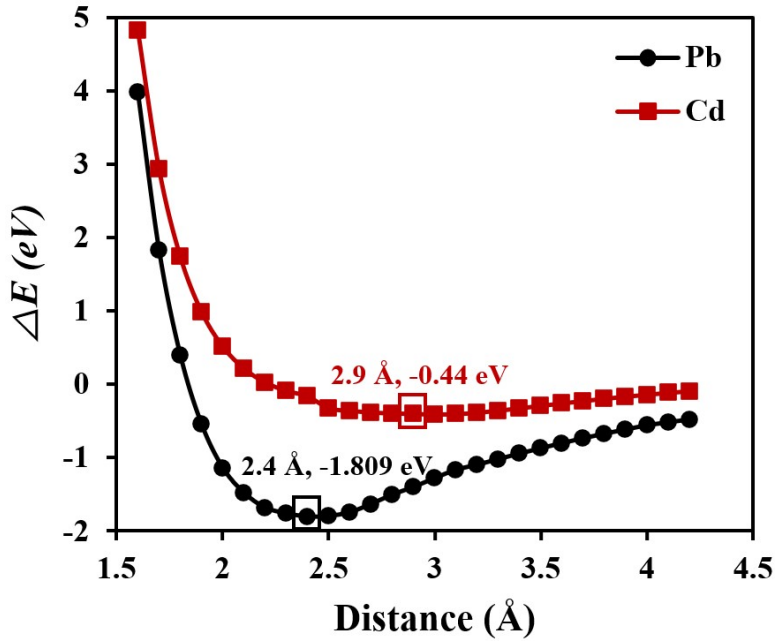

Fig. S2. Plot of DFT calculated lowest binding energy values at different distances for Pb(II) and Cd(II) ions on Nb_2CT_x surface.

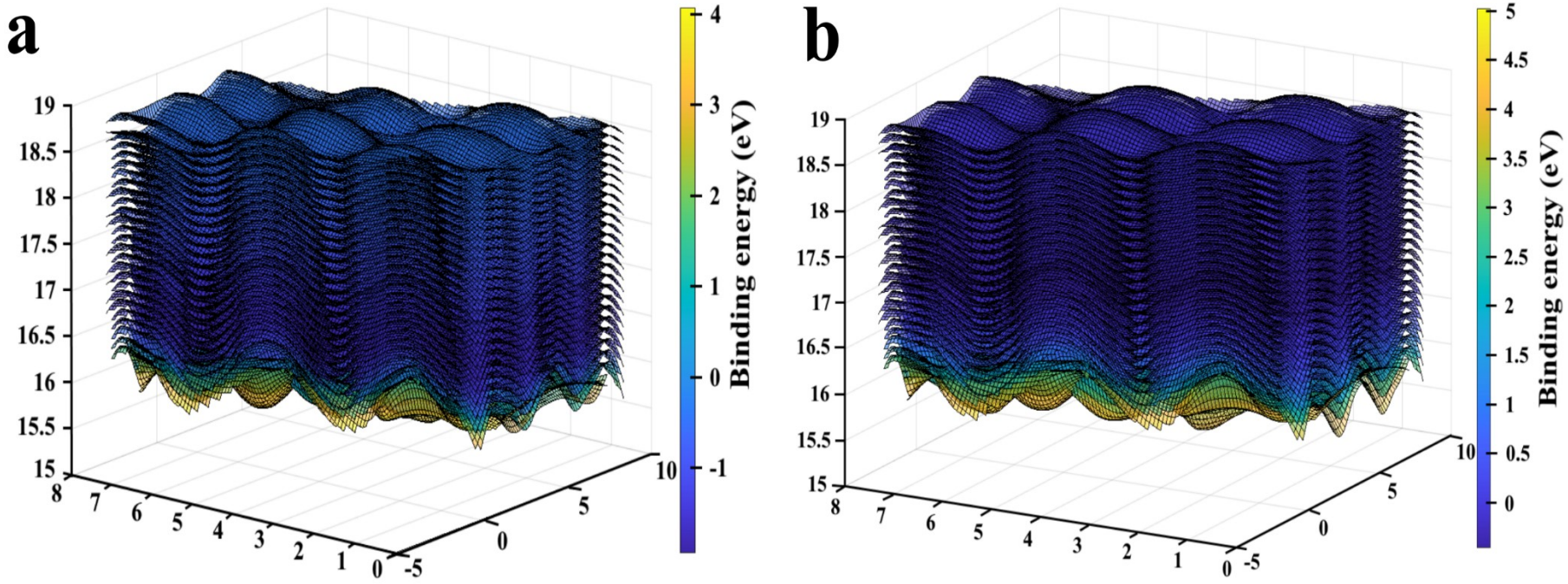

Fig. S3. Predicted binding energy surfaces at different distances from the surface of Nb_2CT_x for (a) Pb(II) ions and (b) Cd(II) ions.

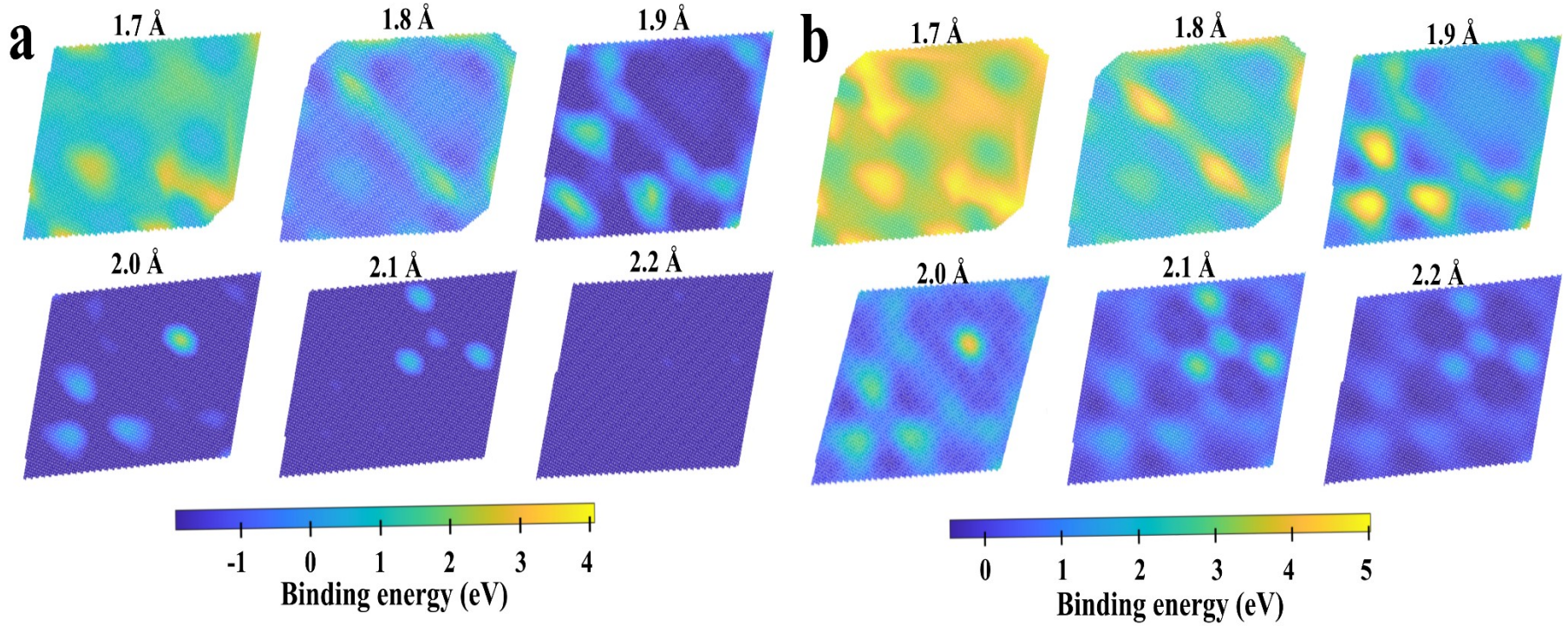

Fig. S4. Top views of the predicted adsorption energy surfaces at different distances from Nb_2CT_x structure for (a) Pb(II) ions and (b) Cd(II) ions.

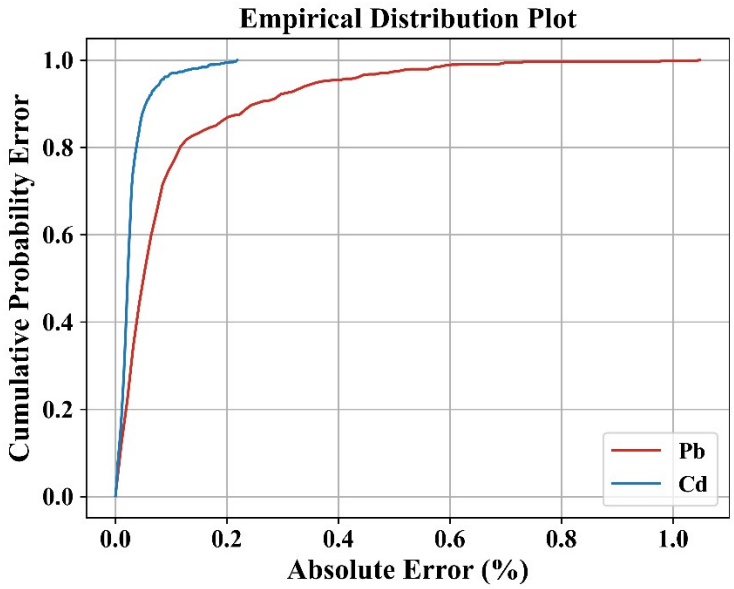

Fig. S5. EDP plot for binding energies of the CGCNN model.

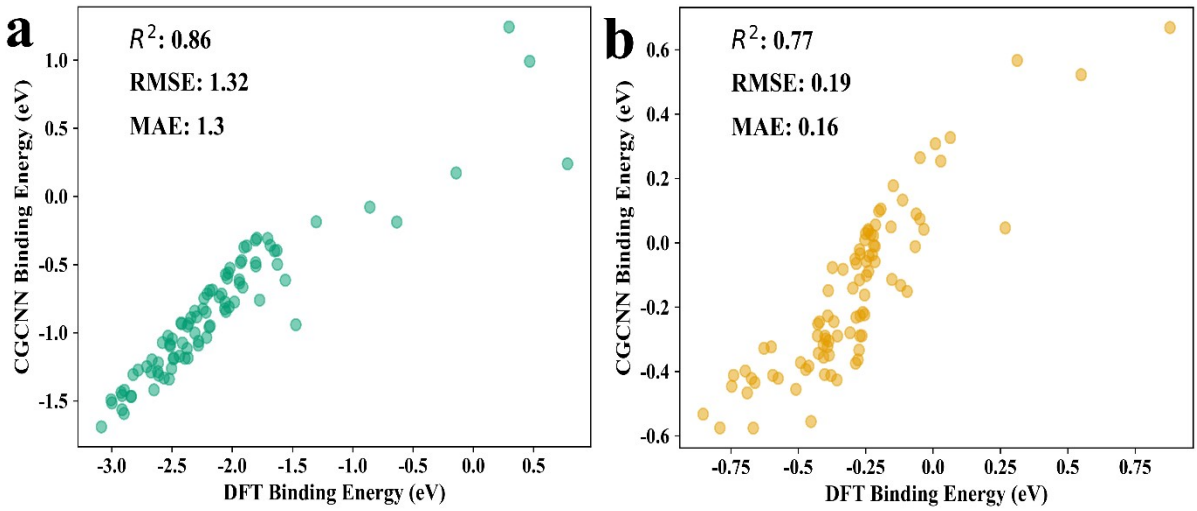

Fig. S6. Comparison between DFT calculated and CGCNN predicted adsorption energies for surface-defected Nb_2CT_x (a) Pb(II) and (b) Cd(II) ions.

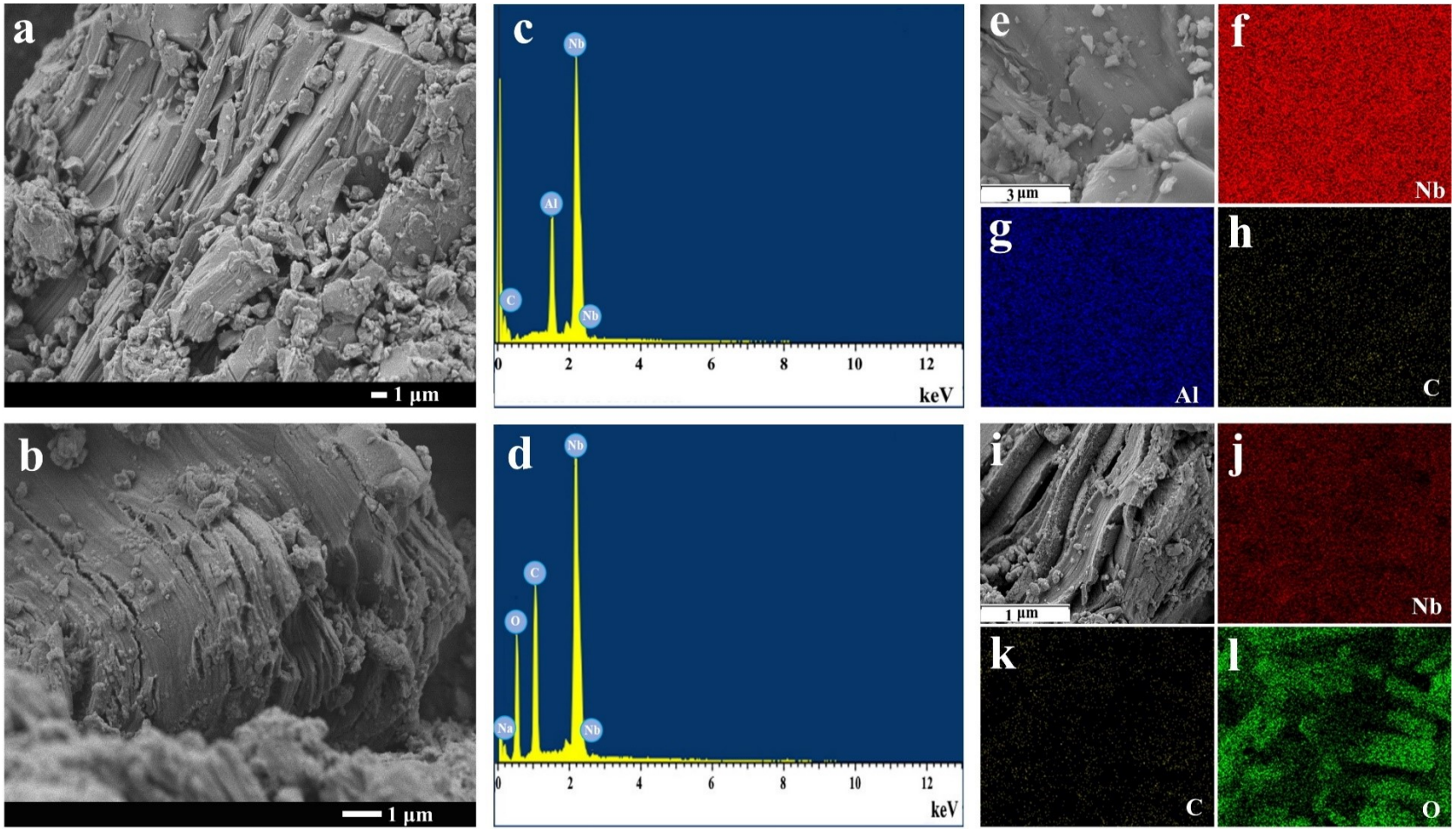

Fig. S7. FESEM analysis of (a) Nb_2AlC, (b) Nb_2CT_x samples, EDX analysis of (c) Nb_2AlC and (d) Nb_2CT_x samples, EDX elemental mapping of Nb_2AlC (e) SEM image of selected region, (f) Nb, (g) Al, (h) C element, and EDX elemental mapping of Nb_2CT_x (i) SEM image of selected region (j) Nb, (k) C and (l) O element.

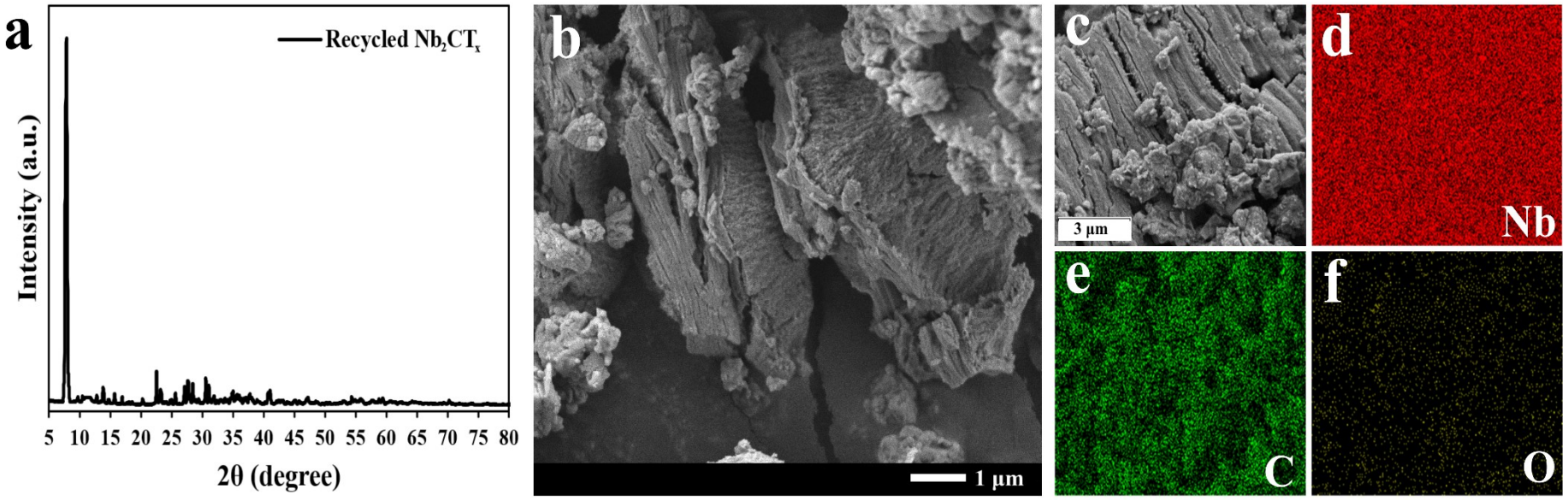

Fig. S8. (a) XRD patterns of the recycled Nb_2CT_x and (b) FESEM image of recycled Nb_2CT_x, EDX mapping of recycled Nb_2CT_x (c) SEM image of selected region (d) Nb, (e) C and (f) O element.

Table S1: Hyperparameters of the CGCNN model

Hyperparameters	Ranges
epochs	100
Batch size	16
Learning rate	0.001
Number of hidden atom features in the convolution layers	64
Number of convolution layers	3
Number of hidden features after pooling	1
Regularization term λ[a]	e^{-6}, e^{-4}, e^{-2}, e^{-0}

a L2 regularization term $\lambda^{\|W\|_2^2}$ is inserted to cost function to decline the overfitting.