Supporting Information for
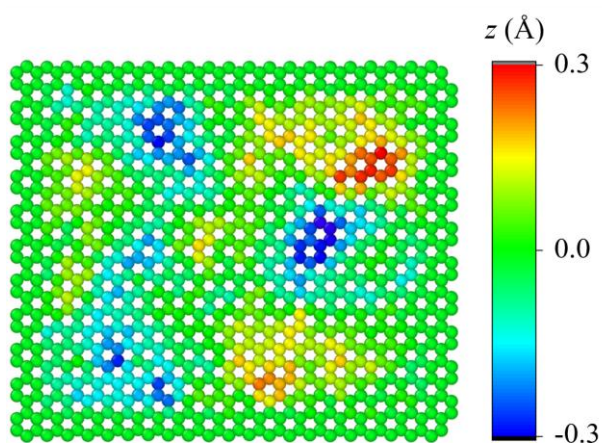
Machine Learning-Based Detection of Graphene Defects with Atomic Precision

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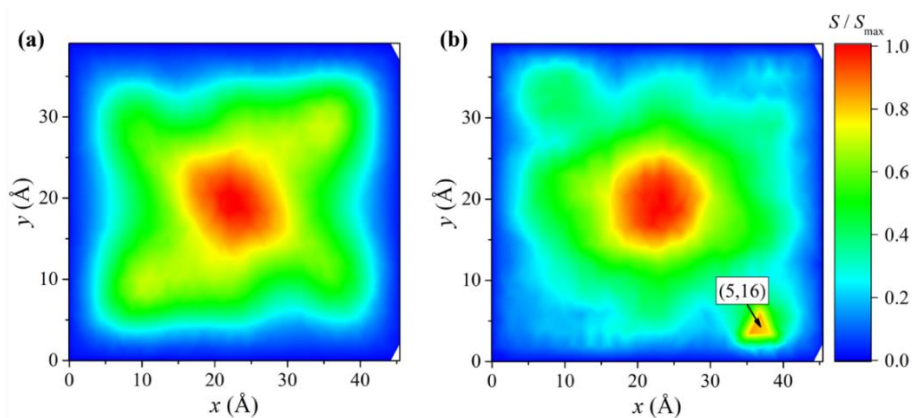
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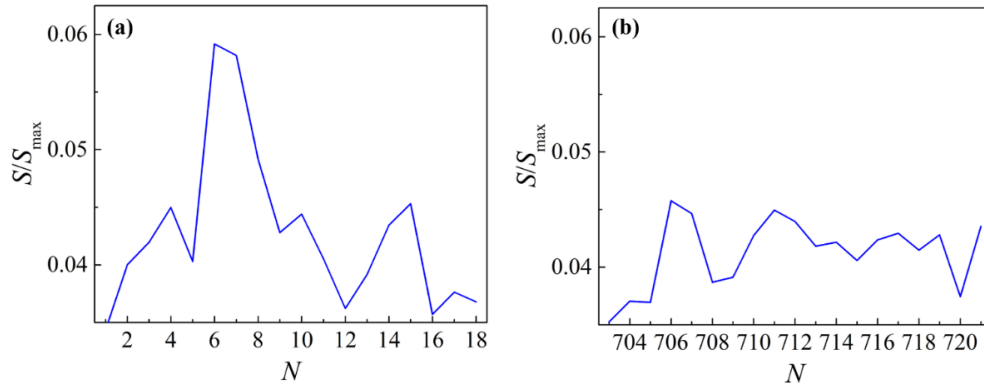
Supplementary Figures

**Fig. S1** Distribution of atom out-of-plane displacement during the thermal vibration of a pristine graphene sheet

**Fig. S2** 2D energy distributions of (**a**) a pristine graphene sheet and (**b**) a graphene sheet with a vacancy (5, 16)

Fig. S3 Portions of energy vector corresponding to (**a**) the first row and (**b**) the last row of atoms. The graphene sheet here contains a single vacancy at (1,10), which lies on the first row of atoms
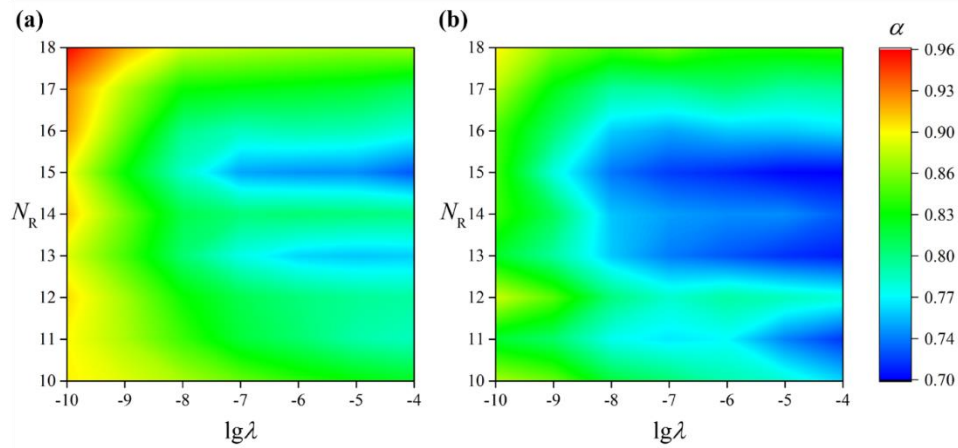
Fig. S4 Effect of regularization on predicting a single-atom vacancy by the domain-based method. (**a**) Validation and (**b**) testing accuracies as a function of N_R and λ
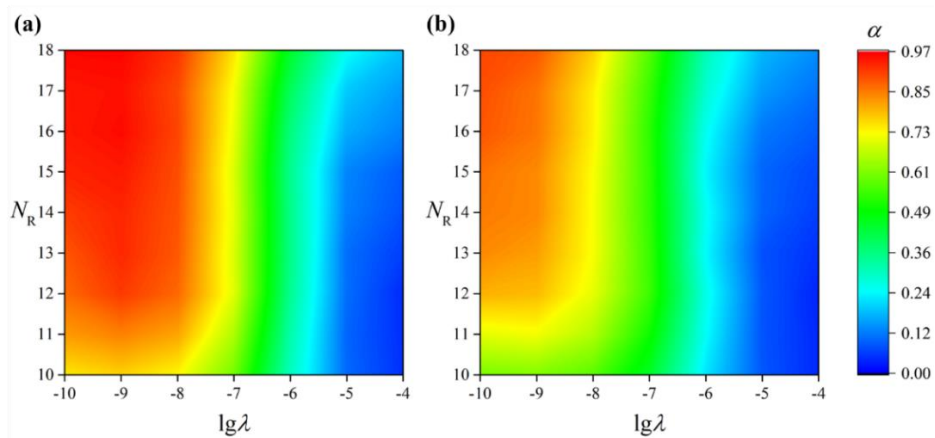
Fig. S5 Effect of regularization on predicting multiple vacancies by the domain-based method. (**a**) Validation and (**b**) testing accuracies as a function of N_R and λ, with $\tau = 0.4$