Supporting Information

Deep Learning of Atomically Resolved Scanning Transmission Electron Microscopy Images: Chemical Identification and Tracking Local Transformations

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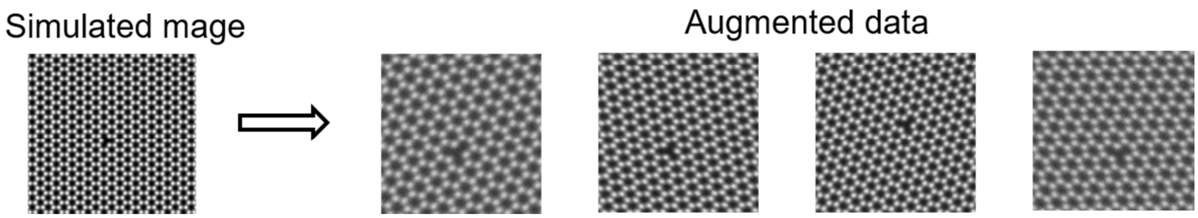
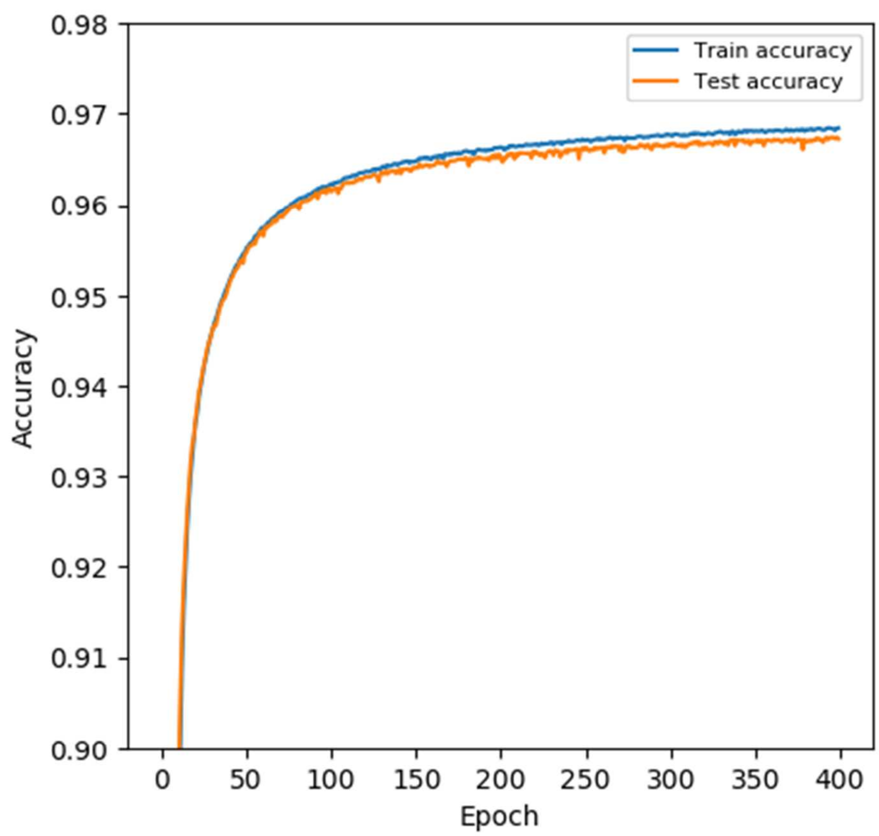
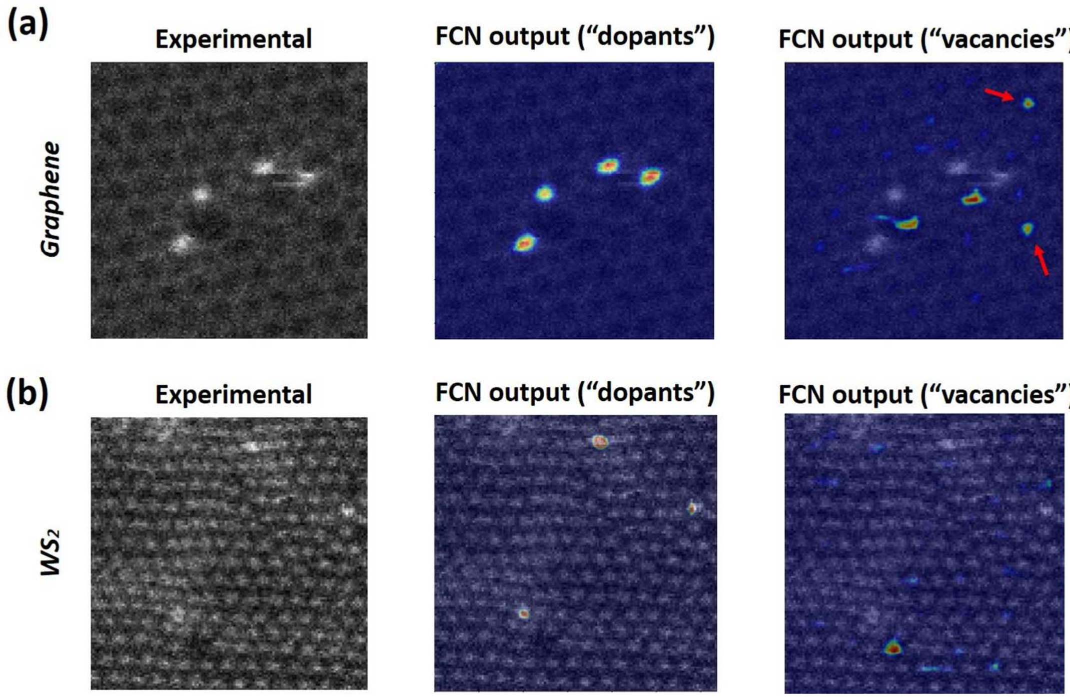


Supplementary Figure 1. Illustration of data augmentation procedure for creating a sufficiently large training set.



Supplementary Figure 2. Plots of accuracy on the training and validation datasets over training epochs for FCN trained for finding atoms in the lattice. The accuracy on the test set is close to 97 %. The FCNs for finding vacancies and dopants typically achieve about 99 % accuracy.



Supplementary Figure 3. Detection of vacancies and vacancy-like structures in graphene and WS_2. (a) Original experimental image and the softmax outputs overlaid on the experimental image. Arrows denote regions that break lattice symmetry due to formation of 5-7 reconstruction and are characterized by extended darker regions (in a region with heptagon). (b) Same for WS_2. See Supplementary Note 1 for additional details.

Supplementary Note 1

To illustrate how the FCN network searches for "dopants" (with higher *Z*) and "vacancies" we show in Supplementary Figure 3 the relevant FCN outputs for graphene and WS_2. In the case of graphene (Supplementary Figure 3a), in addition to identifying areas where carbon atoms are missing, the network also identifies areas that break lattice symmetry due to formation of 5-7 reconstruction and are characterized by extended hollow regions for a heptagon (denoted by red arrows).

In the case of WSe_2, the STEM image shows a large asymmetry between two sublattice sites on the honeycomb lattice effectively turning it into a trigonal lattice. Remarkably, the neural network that learned a concept of dopant (with higher Z) and vacancy on one type of the lattice structure, can apply it to a different lattice, which is very similar to the way a human would do it.