Supporting Information Lattice Convolutional Neural Network Modelling of Adsorbate Coverage-Effects

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Section S1. Residual Plots



Figure S1. Residual plots showing the performance of the heuristic-assisted cluster expansion for all iterations using 90% of the data for training and the remainder for testing. Colors indicate the relative coverage of O (red), vacancies (green), and NO (blue). Left shows the training data. Right shows the test data.





Figure S2. Residual plots showing the performance of the GA-assisted cluster expansion for all iterations using 90% of the data for training and the remainder for testing. Colors indicate the relative coverage of O (red), vacancies (green), and NO (blue). Left shows the training data. Right shows the test data.





Figure S3. Residual plots showing the performance of the LASSO-assisted cluster expansion for all iterations using 90% of the data for training and the remainder for testing. Colors indicate the relative coverage of O (red), vacancies (green), and NO (blue). Left shows the training data. Right shows the test data.





Figure S4. Residual plots showing the performance of the Crystal Graphical Convolutional Neural Network for all iterations using 90% of the data for training and the remainder for testing. Colors indicate the relative coverage of O (red), vacancies (green), and NO (blue). Left shows the training data. Right shows the test data.





Figure S5. Residual plots showing the performance of the Lattice Convolutional Neural Network for all iterations using 90% of the data for training and the remainder for testing. Colors indicate the relative coverage of O (red), vacancies (green), and NO (blue) for one iteration using 90% of the data for training and the remainder for testing. Left shows the training data. Right shows the test data.



Section S2. Visualization of the Lattice Convolutional Neural Network

Figure S6. (a) First, (b) second and (c) third eigenspace values of the site layer after one convolution (red, green and blue colors from Figure 4b) split and plotted as heat maps.



Figure S7. First, second, and third eigenspace extracted from the configuration shown in Figure 4c, and d, and transformed to the heatmap after the second convolutions and the sitewise activation layers.



Figure S8. Eigenspace heatmap throughout the model and site contributions heatmap of two NO molecules separated by increasing distance.



Figure S9. Site formation energy visualization of ground state configurations predicted by PBE and PBE-D3 at 0.42 ML O and 0.42 ML NO. Colors indicate the site formation energy in eV. Two models show the highest disparity in formation energies at this coverage among common ground state convex hull coverages.