

AUTHOR CORRECTION OPEN



Author Correction: Graph neural networks for an accurate and interpretable prediction of the properties of polycrystalline materials

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npj Computational Materials (2022)8:122; <https://doi.org/10.1038/s41524-022-00804-9>

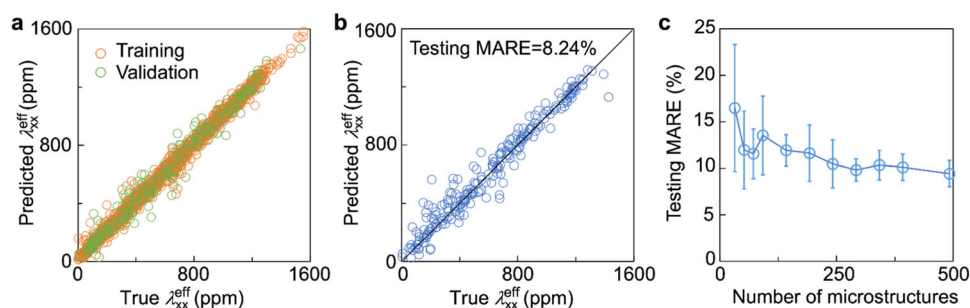
Correction to: npj Computational Materials <https://doi.org/10.1038/s41524-021-00574-w>, published online 09 July 2021.

The authors became aware that the message passing (via the term $\hat{D}^{-\frac{1}{2}}\hat{A}\hat{D}^{-\frac{1}{2}}$) between neighboring nodes was not implemented in the layer-wise update function (Equation (1)) due to an error in the original code of the graph neural network (GNN) model. After code modification, the following changes have been made to the original version of this Article:

Figure 4 depicts the property prediction by the trained GNN model. The correct version of Figure 4 appears below:

The sixth sentence of the first paragraph of the “Property prediction by the GNN model” section originally stated “The MARE for these data is as low as 8.05%”. In the corrected version, “as low as 8.05%” is replaced by “as low as 8.24%”.

The tenth sentence of the first paragraph of the “Property prediction by the GNN model” section originally stated “As shown in Fig. 4c, the average value of the MARE quickly decreases from 17% to ~10%”. In the corrected version, “17% to ~10%” is replaced by “~16% to ~12%”.



which replaces the previous incorrect version, given below:

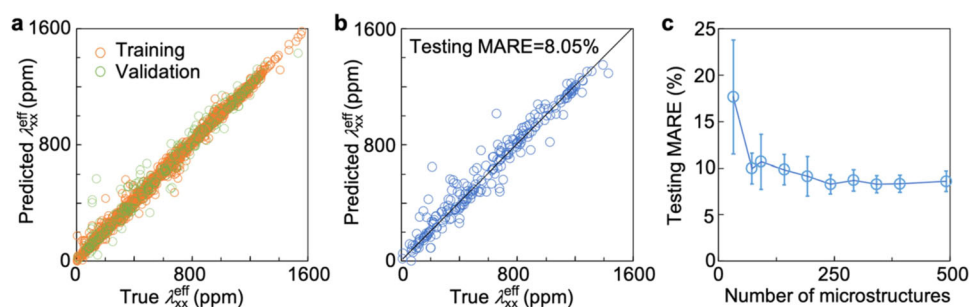
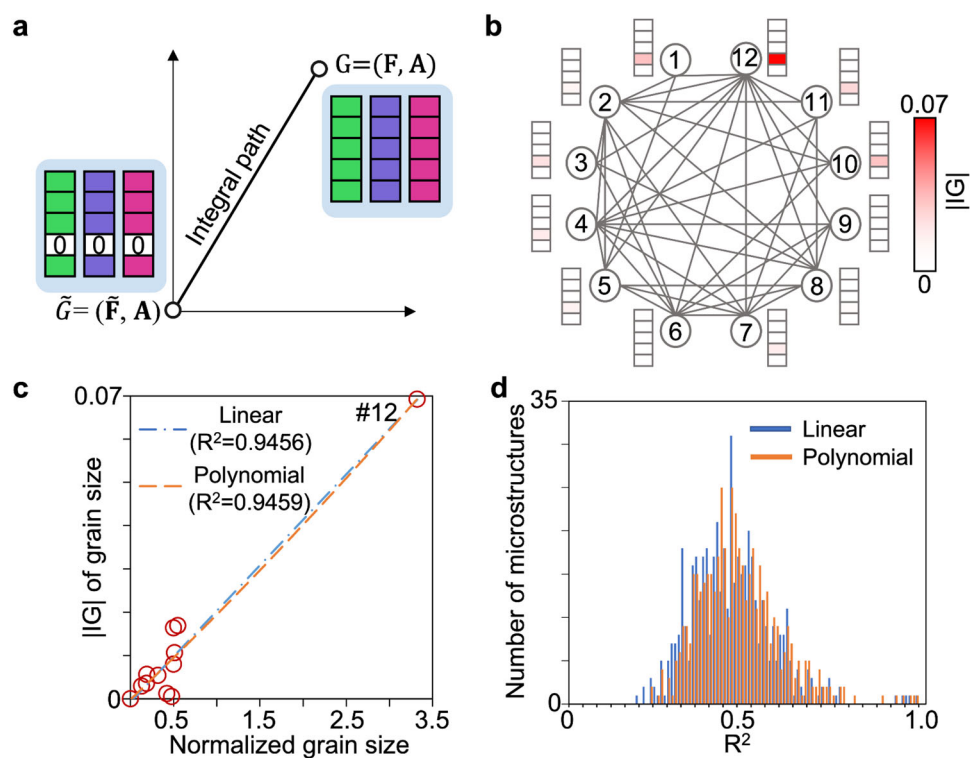
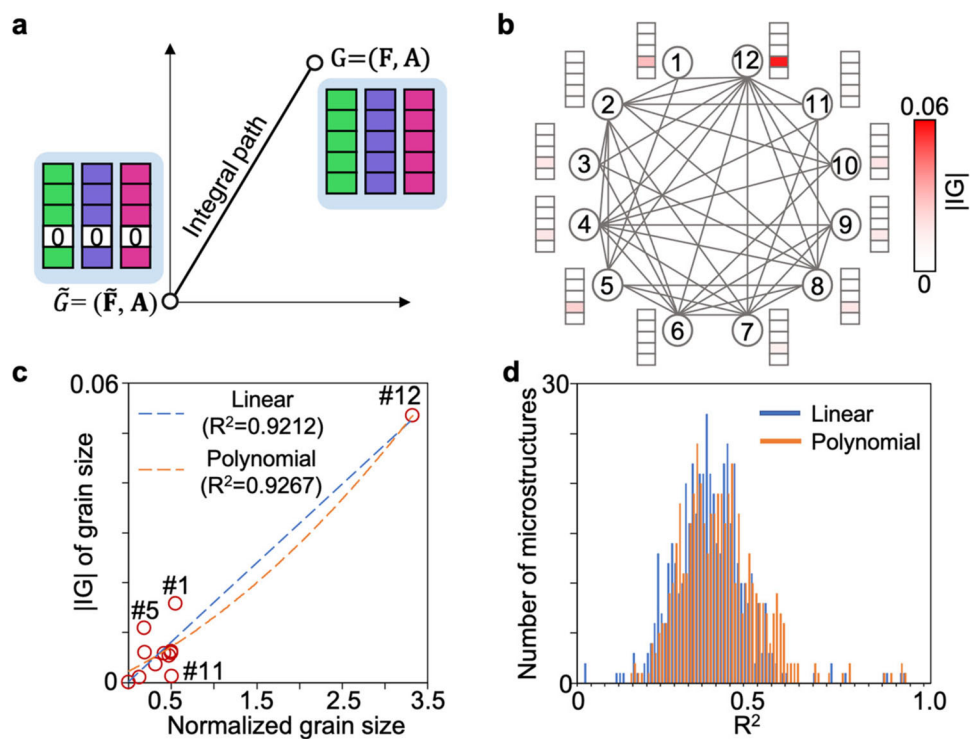


Figure 6 depicts the integrated gradient (IG) analysis. The correct version of Figure 6 appears below:



Which replaces the previous incorrect version, given below:



The second sentence of the fourth paragraph of the Discussion originally stated “the GNN model demonstrates a low relative error of 8.05% in property prediction”. In the corrected version, “a low relative error of 8.05%” is replaced by “a low relative error of 8.24%”.


In Table 1, the values for $W^{(2)}$ and number of epochs were updated. The correct version of Table 1 appears below:

Table 1. Hyperparameters of the optimized GNN model.						
$W^{(1)}$	$W^{(2)}$	N_{h1}	N_{h2}	Batch size	Number of epochs	Learning rate
5×60	60×3	1024	128	32	2000	1×10^{-4}

Which replaces the previous incorrect version:

Table 1. Hyperparameters of the optimized GNN model.						
$W^{(1)}$	$W^{(2)}$	N_{h1}	N_{h2}	Batch size	Number of epochs	Learning rate
5×60	60×5	1024	128	32	1000	1×10^{-4}

The changes have been made to both the PDF and HTML versions of the Article.



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