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Author Correction: Atomistic Line Graph Neural Network for improved materials property predictions

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Correction to: *npj Computational Materials* https://doi.org/10.1038/s41524-021-00650-1, published online 15 November 2021

The original version of this Article contained errors in values of ALIGNN data in Table 5. As a result, the following changes have been made to the original version of this Article:

In Table 5, the data for "OrbNetens5" column were removed and values for "ALIGNN" column were updated. The correct version of Table 5 appears below:

Table 5. Regression model performances on QM9 dataset for 11 properties using ALIGNN.

Target	Units	SchNet	MEGNet	DimeNet++	ALIGNN
HOMO	eV	0.041	0.043	0.0246	0.0214
LUMO	eV	0.034	0.044	0.0195	0.0195
Gap	eV	0.063	0.066	0.0326	0.0381
ZPVE	eV	0.0017	0.00143	0.00121	0.0031
μ	Debye	0.033	0.05	0.0297	0.0146
α	$Bohr^3$	0.235	0.081	0.0435	0.0561
R^2	$Bohr^2$	0.073	0.302	0.331	0.5432
U0	eV	0.014	0.012	0.00632	0.0153
U	eV	0.019	0.013	0.00628	0.0144
H	eV	0.014	0.012	0.00653	0.0147
G	eV	0.014	0.012	0.00756	0.0144

These models were trained with same parameters as solid-statedatabases but for 1000 epochs. Predictions on test set are shownin Supplementary Fig. S42 to Supplementary Fig. S52.

Which replaces the previous incorrect version:

Table 5. Regression model performances on QM9 dataset for 11 properties using ALIGNN.

Target	Units	SchNet	MEGNet	DimeNet++	OrbNet-ens5	ALIGNN
HOMO	eV	0.041	0.043	**0.0246**	—	0.037
LUMO	eV	0.034	0.044	0.0195	—	**0.016**
Gap	eV	0.063	0.066	0.0326	—	**0.030**
ZPVE	eV	0.0017	0.00143	**0.00121**	—	0.002
μ	Debye	0.033	0.05	0.0297	—	**0.018**
α	$Bohr^3$	0.235	0.081	0.0435	—	**0.008**
$<R^2>$	$Bohr^2$	0.073	0.302	0.331	—	**0.002**
U0	eV	0.014	0.012	0.00632	0.0039	**0.00209**
U	eV	0.019	0.013	0.00628	—	**0.00181**
H	eV	0.014	0.012	0.00653	—	**0.00237**
G	eV	0.014	0.012	0.00756	—	**0.00226**

Predictions on test set are shown in Supplementary Figs. 42–52. The bold values represent the best performing models.

Consequently, the last sentence in Abstract was stated "ALIGNN can outperform some previously reported GNN models on atomistic prediction tasks by up to 85% in accuracy with better or comparable model training speed." In the corrected version, "by up to 85% in accuracy" was omitted.

The first sentence of the last paragraph of the "Model Performance" section originally stated "Next, we evaluate the ALIGNN model on QM9 molecular property dataset (130,829 molecules) and compare it with other well-known models such as SchNet[10], MatErials Graph Network (MEGNet)[16], OrbNet[18], and DimeNet++[20] as shown in Table 5." In the corrected version, "OrbNet[18]," was omitted.

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A new sentence "The results from models other than ALIGNN are reported as given in corresponding papers, not necessarily reproduced by us." was inserted after the first sentence of the last paragraph of the "Model Performance" section.

The fourth sentence of the last paragraph of the "Model Performance" section originally stated "ALIGNN outperforms competing methods on 9 out of 11 tasks, suggesting that it can be uniformly applied to both molecular as well as solid-state systems. On the QM9 U0 regression target, ALIGNN outperforms SchNet, MEGNet, DimeNet++ and OrbNet by 85%, 82.3%, 66.8%, and 46.2% respectively." In the corrected version, the sentence stated "ALIGNN outperforms competing methods for HOMO and dipole moment tasks while other accuracies are similar to the SchNet model.".

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