

Peer Review Information

Journal: Nature Computational Science

Manuscript Title: Virtual Node Graph Neural Network for Full Phonon Prediction

Corresponding author name(s): Professor Mingda Li

Editorial Notes:

Transferred manuscripts This manuscript has been previously reviewed at another journal that is not operating a transparent peer review scheme. This document only contains reviewer comments, rebuttal and decision letters for versions considered at Nature Computational Science

Reviewer Comments & Decisions:

Decision Letter, initial version:
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Date: 8th December 23 03:01:36

Last Sent: 8th December 23 03:01:36

Triggered By: Jie Pan

From: jie.pan@us.nature.com

To: mingda@mit.edu

BCC: jie.pan@us.nature.com

Subject: Decision on Nature Computational Science manuscript NATCOMPUTSCI-23-1680-T

Message: Dear Professor Li,

Thank you for submitting "Virtual Node Graph Neural Network for Full Phonon Prediction" to Nature Computational Science, and we apologize for the delay in reaching a decision on your manuscript. Regretfully, we cannot offer to publish it.

In this case, we have no doubt that your virtual node graph neural network and its application in phonon calculations will be of interest to fellow experts in computational materials science. While we've found your work is potentially interesting and agreed to further consider a suitable revised version that properly addresses the review

comments from Nature, I regret that we are unable to conclude that the revision together with the new benchmark results provides the sort of substantial practical or conceptual advance that would be of immediate interest to a broad readership of researchers in computational science. Specifically, this revision does not present enough substantial advance when compared to existing deep-learning methods, such as M3GNet, in phonon calculation tasks, and thus, it is unclear on what can be done differently with your methods. Therefore, although we do not doubt that the advantages of your method are worth publishing in a more specialist journal – such as npj Computational Materials, we are not convinced that they deserve the high visibility of a Nature Computational Science publication.

Although we cannot offer to publish your manuscript, I suggest that you consider npj Computational Materials as a suitable venue for this work. To transfer your manuscript, please use our [REDACTED] You will not have to re-supply manuscript metadata and files, unless you wish to make modifications. For more information, please see our [manuscript transfer FAQ](#) page.

I am sorry that we cannot respond more positively, and I hope you will understand that our decision in no way reflects any questions about the quality of the work reported. Again, we apologize for the delay in reaching a decision on your manuscript, and we hope you will rapidly receive a more favorable response elsewhere.

Best regards,

Jie Pan, Ph.D.
Senior Editor
Nature Computational Science

For Nature Portfolio general information and news for authors, see <https://www.nature.com/nature-research/for-authors>.

Decision Letter, first revision:

Date: 23rd February 24 12:08:37

Last Sent: 23rd February 24 12:08:37

Triggered By: Jie Pan

From: jie.pan@us.nature.com

To: mingda@mit.edu

BCC: jie.pan@us.nature.com

Subject: Decision on Nature Computational Science manuscript NATCOMPUTSCI-23-1680A-Z

Message: Dear Professor Li,

Thank you for your correspondence asking us to reconsider our decision on your

Article, "Virtual Node Graph Neural Network for Full Phonon Prediction". Now that I have had a chance to discuss the matter carefully with my colleagues, I am sorry to have to tell you that we do not feel able to reverse our original decision. Sorry for the delay in getting back to you, since the week of Feb 12th was a holiday week for our Shanghai based staff. Thank you for the patience.

We appreciate your response to the points raised in review, as well as the revision according to our discussion. However, we feel it is unlikely that the referees will change their overall view of the work in the light of your reply, especially on the point of the advance beyond the phonon band calculation with molecular dynamics and machine learning interatomic potentials, and we can see little to be gained by sending the paper back out to review. We continue to feel that your paper would find a more suitable outlet in another journal rather than Nature Computational Science.

Should future experimental data allow you to address the following point, we would be happy to look at a revised manuscript and reassess the work to decide whether or not we will send it out to peer review (unless, of course, something similar has by then been accepted at Nature Computational Science or appeared elsewhere). This includes submission or publication of a portion of this work somewhere else. In the case of eventual publication, the received date would be that of the revised paper.

- Please clearly demonstrate the advance in a broader context, not limiting to conventional GNN with zero padding technique. For instance, although the accuracy is similar, you could provide comparisons against molecular dynamics simulations with machine learning interatomic potentials to show advance in computational efficiency (e.g., cost and memory).

In addition, editorially we feel that VGNN can potentially be an useful tool to generate datasets, on the condition that you can demonstrate the above point. The database containing 146k materials might be of interest to materials informatics community. Given these in consideration, we feel that your manuscript is more suited as a Resource rather than an Article for our journal. The formats of Resource and Article are similar, and please find more information about our content types at <https://www.nature.com/natcomputsci/content>.

If you are interested in submitting a suitably revised manuscript in the future or if you have any questions, please contact me. In case you are not interested in submitting a revised version, you may transfer your manuscript to another journal in the Nature Portfolio using the link I provide at the end of this email.

I am sorry that we cannot be more positive on this occasion. Unfortunately, the number of papers submitted to Nature Computational Science vastly exceeds the number that we can publish each month, and we are therefore frequently forced to make difficult decisions. Should you have questions, please let me know.

Best regards,

Jie Pan, Ph.D.
Senior Editor
Nature Computational Science

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Decision Letter, second revision:
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Date: 10th May 24 10:42:35
Last Sent: 10th May 24 10:42:35
Triggered By: Jie Pan
From: jie.pan@us.nature.com
To: mingda@mit.edu
CC: computacionalscience@nature.com
BCC: jie.pan@us.nature.com
Subject: AIP Decision on Manuscript NATCOMPUTSCI-23-1680B-Z
Message: Our ref: NATCOMPUTSCI-23-1680B-Z

10th May 2024

Dear Dr. Li,

Thank you for submitting your revised manuscript "Virtual Node Graph Neural Network for Full Phonon Prediction" (NATCOMPUTSCI-23-1680B-Z). It has now been seen by the original referees and their comments are below. The reviewers find that the paper has improved in revision, and therefore we'll be happy in principle to publish it in Nature Computational Science, pending minor revisions to satisfy the referees' final requests and to comply with our editorial and formatting guidelines.

We are now performing detailed checks on your paper and will send you a checklist detailing our editorial and formatting requirements in about 10 days. Please do not upload the final materials and make any revisions until you receive this additional information from us.

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Thank you again for your interest in Nature Computational Science. Please do not hesitate to contact me if you have any questions.

Sincerely,

Jie Pan, Ph.D.
Senior Editor
Nature Computational Science

ORCID

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Reviewer #2 (Remarks to the Author):

The authors have considerably improved the manuscript performing an important amount of new calculations. I still have a few minor concerns that should be addressed before publication.

In their comparison with respect to M3GNet, the authors indicate "The average loss over the test data is presented in Table 2, with more details mentioned in Supplementary Information VI." It is not clear to me which part of section VI of the Supplementary Information they are referring to. How many materials were considered for computing the loss? This information should be mentioned in the manuscript. Why don't they report MAE values (with the corresponding units)?

Also, in the meantime, we have performed a systematic assessment of various universal MLIPs (<https://arxiv.org/abs/2403.05729>). In our case, 101 materials were selected and various metrics have been used to characterize the errors. And, it seems that MACE is providing better results than M3GNet (even though a new version of M3GNet is available). I am not asking the authors to perform any new calculations. As indicated above, I would like to get the MAEs (or at the very least to understand how the loss is computed). Furthermore, it would be nice to indicate that other universal MLIPs exist and their performance can (or could) be better than M3GNet...

Author Rebuttal, Second revision:

Response to the reviewers' comments on our accepted paper "Virtual Node Graph Neural Network for Full Phonon Prediction"

We sincerely appreciate your thorough review and valuable comments on our manuscript. Your feedback has been instrumental in enhancing the clarity and quality of our work. Please find our detailed responses to your comments below:

Reviewer 2's comments

- (1) In their comparison with respect to M3GNet, the authors indicate "The average loss over the test data is presented in Table 2, with more details mentioned in Supplementary Information VI." It is not clear to me which part of section VI of the Supplementary Information they are referring to. How many materials were considered for computing the loss? This information should be mentioned in the manuscript. Why don't they report MAE values (with the corresponding units)?

We have revised the manuscript to explicitly mention that the comparison of our new method (k-MVN) with existing methods, including M3GNet, is detailed in Supplementary Information 6.5. In Supplementary Information 6.5, we specify that the Main Database of 1.5k materials, each with phonon band structure data, was used to compute the loss. This information has now been included in the main manuscript for better clarity. Additionally, we have computed the Mean Absolute Error (MAE) with and without normalization on the input values. The results are presented in Table S6 of the Supplementary Information, along with the corresponding units for the MAE values to ensure clarity and precision.

- (2) Also, in the meantime, we have performed a systematic assessment of various universal MLIPs (<https://arxiv.org/abs/2403.05729>). In our case, 101 materials were selected and various metrics have been used to characterize the errors. And, it seems that MACE is providing better results than M3GNet (even though a new version of M3GNet is available). I am not asking the authors to perform any new calculations. As indicated above, I would like to get the MAEs (or at the very least to understand how the loss is computed). Furthermore, it would be nice to indicate that other universal MLIPs exist and their performance can (or could) be better than M3GNet...

We have acknowledged the existence of other universal Machine Learning Interatomic Potentials (MLIPs), including MACE, both in the manuscript and in the Supplementary Information. As previously mentioned, the MAE results are presented in Table S6 of the Supplementary Information. This includes detailed information on how the loss is computed. We appreciate the reference to the systematic assessment of various universal MLIPs and acknowledgments. We have noted this in the manuscript to provide a comprehensive overview of the current state of MLIPs and their performance metrics.

Final Decision Letter:

Date: 13th June 24 12:55:03

Last Sent: 13th June 24 12:55:03

Triggered By: Jie Pan

From: jie.pan@us.nature.com

To: mingda@mit.edu

BCC: jie.pan@us.nature.com, computacionalscience@nature.com, rjsproduction@springernature.com, fernando.chirigati@us.nature.com

Subject: Decision on Nature Computational Science manuscript NATCOMPUTSCI-23-1680C

Message: Dear Professor Li,

We are pleased to inform you that your Article "Virtual Node Graph Neural Network for Full Phonon Prediction" has now been accepted for publication in Nature Computational Science.

Once your manuscript is typeset, you will receive an email with a link to choose the appropriate publishing options for your paper and our Author Services team will be in touch regarding any additional information that may be required.

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We look forward to publishing your paper.

Best regards,

Jie Pan, Ph.D.
Senior Editor
Nature Computational Science

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