**Response to the Reviewers**

We are grateful to the Reviewer for the valuable suggestions and comments. We have carefully considered all comments and suggestions and have revised the manuscript accordingly.

**Reviewer(s)' Comments to Author:**

**Reviewer: 1**  
Comments to the Author

The authors present their TensorFlow-based program for training and predicting potential energies, forces, and virial stress of atomistic (materials) systems. The code is clean and understandable.  The methods are explained well and are understandable. The machine learning and science used to develop the code is well established, except perhaps the ability to train the model to the virial stress, which I have not found within any other ML framework implemented ML potential. This ability represents a new addition to the community. Although, several ML frameworks provide the ability to simply predict (not train to) virials, which is trivial once you obtain forces with AutoGrad in any ML framework. 

1. Please make it more clearly in the introduction that your code allows virial training. Any potential readers have to the read the paper in depth to find where it is explicitly stated. I had to go all the way to the methods to find an explicit statement to this end. It seems to be hinted to in the abstract and intro. The virial training part is what sets the code apart from the rest of the pack. For example, in the abstract you say: "To precisely describe complex potential energy surfaces, integrating advanced metrics, such as force or virial stress, into training can be of great help". However, the abstract does NOT clearly state that your code does this. You simply say: "Our approach creates the computation graph directly from atomic positions. Thus, the derivations of forces and virial can be handled by TensorFlow automatically and efficiently." This is exactly what someone trying to simply predict forces and virials would say and does not imply force and virial training.   
   Maybe add a sentence like: "The virtual atom approach with auto grad within TensorFlow allows for efficient training to not just energies and forces, but also virial stress." The conclusions also fail to mention this important feature.

***Authors’ response:*** *Thanks very much for your suggestion. We have slightly improved our abstract and introduction to make this clear.*

1. Some discussion or results on how well virial stress can be predicted with only energy and force training would be a great addition to backup any arguments on why you need to use virial training. I am not fully convinced it is necessary to use virial training since force training can provide very low errors, and the virial is completely based on forces

***Authors’ response:*** *Thanks very much for your comment.*

*From the theoretical point of view, the original virial stress equation proposed by Thompson et al 2009 (Eq. 18 in the manuscript) consists of two parts:*

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*The left part represents the net force contribution (net force on each atom) while the right part is the total contribution of the partial forces (force between two atoms). Our derived virial equation (Eq. 19) does not change the nature of this equation but just uses an alternative form to calculate the overall partial force contribution. However, the forces included in the total loss function are net forces only. The partial forces may be not that accurate.*

*We did a test to show this. We just use the SNAP-Ni dataset. The new training also includes virial stress in the total loss function with set to 160. Other settings were kept the same.*

*The following table shows the energy and force MAEs:*

|  |  |  |
| --- | --- | --- |
|  | *Energy + Force* | *Energy + Force + Stress* |
| *Energy (meV/atom)* | *1.3* | *2.2* |
| *Force (eV/Angstrom)* | *0.038* | *0.046* |

*Below the table compares the MAEs of predicted virial stress (GPa):*

|  |  |  |
| --- | --- | --- |
| *Component* | *Energy + Force* | *Energy + Force + Stress* |
| *xx* | *3.12* | *0.66* |
| *yy* | *3.12* | *0.67* |
| *zz* | *3.15* | *0.70* |
| *yz* | *0.98* | *0.93* |
| *xz* | *0.95* | *0.90* |
| *xy* | *0.99* | *0.93* |
| *(xx+yy+zz)/3* | *2.05* | *0.80* |
| *Overall* | *2.05* | *0.80* |

*The EFS (energy, force, stress) model has slightly worse performances on energy and force predictions but can give much more accurate stress predictions. Better force accuracy (the EF model) may not lead to accurate stress prediction. Hence, including virial stress is necessary.*