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Dr. Prof. Huang

Many thanks for Dr. Yan Li’s kind invitation on March 18, 2020. Here, I am writing to submit our review entitled “**A Machine Learning Method for Material Property Prediction: Example Polymer Compatibility**” for consideration for publication in ***Cell Reports Physical Science***. This manuscript describes original work and is not under consideration by any other journal. All authors approved the manuscript and this submission.

Material research combined with Machine Learning method has received considerable attentions in recent years. Yet, the database construction and property prediction for polymer material remains challenging. In this paper, we report a general Machine Learning method for material property prediction and construct an effective prediction model Half Dense Difference Network (HDDN). We establish a dataset based on literature mining and Natural Language Processing (NLP) technology, which shows the power of Text Data Mining in science research. We design HDDN in the reference of existing chemistry method for polymer compatibility prediction and it achieves impressive classification results and performs better than chemistry methods and other possible competing ML models. Through ablation experiments we explain why our architecture design can work and quantify the contribution of each module. Furthermore, we conduct case study and confidence test to demonstrate the reliability of our model. Interpretability investigation proves that our model can be interpreted with chemistry knowledge, and more details of our model can be investigated as supplement to existing chemistry knowledge.

Therefore, we believe the publication of our results in ***Cell Reports Physical Science*** will attract attentions and benefit many researchers in various areas, especially in material property research paradigm with machine learning.

We have checked the manuscript carefully and agree to submit it in the present form. This manuscript has not been published previously or under consideration for publication elsewhere.

Thank you very much for your consideration.

Best regards.

Sincerely yours,

Jinying Yuan