Paris, 16 September 2020

Dear Editor,

We are pleased to hereby submit our manuscript entitled “Deep learning prediction of glass and melt properties” to *Science.*

The properties of molten rocks and glasses are critical to many disciplines, including glass industry and Earth sciences. Of particular interest is the link between the chemical composition of such materials, their molecular structure and their physical properties. No general model allows predicting such a link. In particular, the complex non-linear variations of thermodynamic properties with melt composition, such as configurational entropy, have been proven to be extremely difficult to reproduce. Here, we show that deep neural networks can predict such quantities for their use in thermodynamic equations. Not limited to this, the deep neural network can also predict physical glass properties like density or refractive index.

The deep learning framework we created and trained takes chemical composition inputs, and returns melt viscosity through five different theories (it is thus “trans-theoretical”), as well as properties such as glass transition temperature, configurational entropy, glass density, glass optical refractive index or even glass Raman spectra. After training, the deep learning framework allows a systematic exploration and quantification of the links between structure (as seen by Raman spectra), chemical composition and properties of two states of silicate materials : glasses and melts. As a demonstration, we applied this idea on alkali aluminosilicate melts, for which an extended experimental dataset of high quality is available. Albeit simple, the study of this system with the deep learning framework already allows tackling practical problems like why silicic volcanoes like Yellowstone (USA) may erupt explosively if the magma is rich in K and Al, as suggested by a study published in Nature in 2017.

This study is considered of high interest to the diverse readers of *Science* because of the importance of the deep learning framework for the systematic exploration, quantification and prediction of material properties. This approach can be transposed to many different fields. No prior discussions have taken place with an editor of *Science* about the work described in this manuscript. The manuscript or related materials is not under consideration elsewhere. We have provided suggestions for reviewers below. We hope that you will consider our manuscript for publication in *Science.*

On behalf of all the authors,

Yours sincerely,

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