Paris, 23 March 2021

Dear Editor,

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

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 physics-guided 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 addressing practical problems, such the relationship between the composition of silicic magmas and the eruptive dynamics of silicic volcanoes like Yellowstone (USA).

This study is considered of high interest to the diverse readers of *Geochimica Cosmochimica Acta* because of the importance of the deep learning framework for the systematic exploration, quantification and prediction of the properties of geologic melts. Beyond volcanology, this approach can be transposed to many different fields. 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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We suggest Sung Keun Lee (Seoul National University), Marc Norman (Australian National University) and Georges Calas (IMPMC) as associate editors for this paper. We also suggest the following reviewers:

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Because of existing conflicts of interests, we ask the editor not to send the manuscript in review to the following people:

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Don B. Dingwell & Kai Uwe Hess, LMU Munich