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**Front Matter**

**Title**

Deep learning trans-theoretical prediction of material properties: application to aluminosilicate glasses and melts

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**In memory of G.N. Greaves**

**Abstract**

Predicting properties of materials like minerals, liquids or glasses represent a critical goal in many disciplines. Among them, geo- and material sciences share a common interest for the properties of aluminosilicate melts that constitute most of Earth's volcanic magmas and lavas, and that can be quenched to produce technological glasses like hand-held devices' screens. While several avenues allow predictions of the properties of those materials, an extended core model linking their chemical composition to their structure and properties, and thus allowing systematic and extended exploration of those links, do not exist to date. Focusing on alkali aluminosilicate melts, this communication shows how thermodynamic theories can be combined with a core deep neural network to build a framework for prediction of melt and glass properties, like viscosity, density, or even Raman signals. Such approach provides a new way to study and unravel the links between chemistry, structure and properties of materials.

**MAIN TEXT**

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**Introduction**

The prediction of the properties of materials represents a cornerstone for many disciplines that aim to solve problems related to material engineering and manufacturing, or to address key questions in the area of physics, chemistry and geosciences. Particular efforts have been deployed to understand how the chemical composition of aluminosilicate melts and glasses affect their structure, and, in turn, their thermodynamic and dynamic properties (e.g., see the reviews of Mysen and Richet, 2005; Le Losq et al., 2019b). Indeed, those materials form the liquid part of magmas, and their viscosity (resistance to movement) directly drives the effusive or explosive character of volcanic eruptions (Dingwell, 1996; Gonnermann et al., 2013; Gonnermann, 2015), and, hence, influence risk mitigation during eruptive crisis. Furthermore, aluminosilicate glasses are used to manufacture technological glasses used in many areas, like as screens of mobile devices. Knowledge and prediction of the properties of aluminosilicate glasses and melts is thus key to solve many material and Earth sciences problems.

**Results**

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