UNDERSTANDING THE COMPOSITIONAL CONTROL ON ELECTRICAL, MECHANICAL, OPTICAL, AND PHYSICAL PROPERTIES OF INORGANIC GLASSES WITH INTERPRETABLE MACHINE LEARNING

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In materials, understanding and predicting the composition–structure–property relationship is the key to developing novel materials. Such predictions are typically hindered by the complex physics happening at different length and time scales, along with the large number of structural and compositional arrangements possible. As an alternative route, data-driven approaches such as machine learning can prove key to predict structure and composition of materials. Herein, using a large database of glasses (> 450,000 compositions) with up to 232 components, we develop machine learning based models for predicting 25 relevant glass properties. Further, employing Shapley additive explanations (SHAP), we demonstrate the role of each of the input component in controlling the glass property quantitatively. Interestingly, we observe that the components may exhibit a coupled effect—presence of one additional component may reverse the performance of another component as in the case of boron anomaly. We show that SHAP can accurately capture these effects thereby providing insights to composition–property relationship and underlying physics. We believe this step towards decoding the glass genome through interpretable machine learning can significantly improve our fundamental understanding on the compositional control of glass properties.

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