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Designing Functional Glasses using Machine Learning

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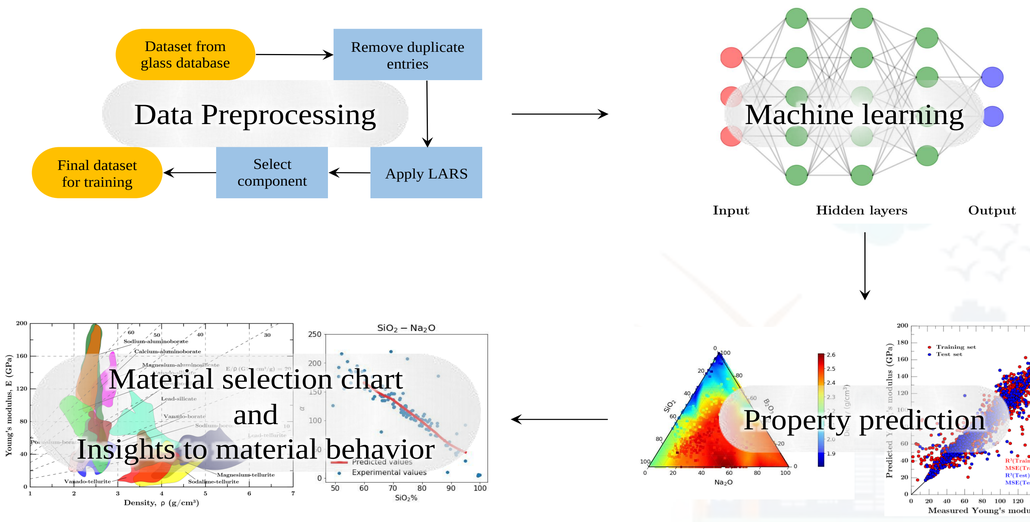
Abstract

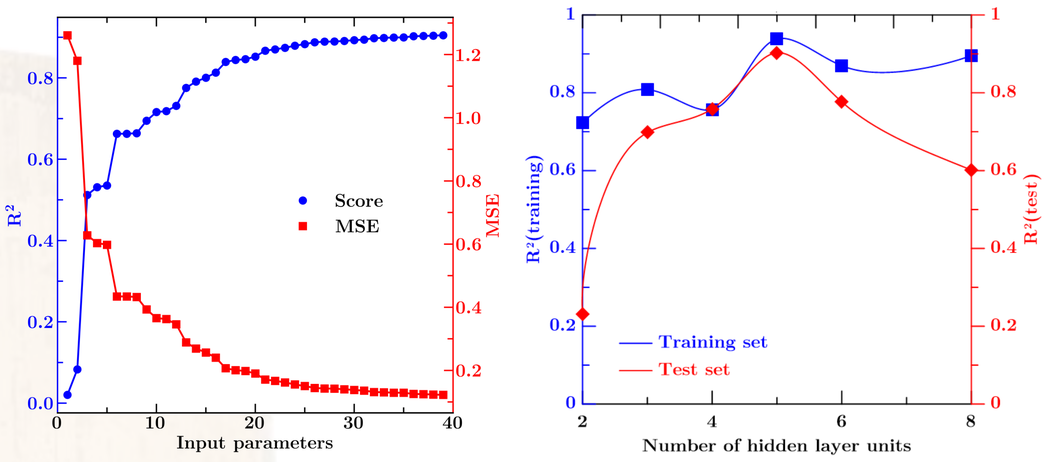
- Inorganic glasses are used in wide range of applications in communication, transportation, healthcare, and nuclear waste immobilization
- These glasses exhibit different properties based on their composition
- There exists infinite number of compositions for inorganic glasses
- **Motivation: Design of functional inorganic glasses for tailored properties**



Methodology

a) Data Preparation

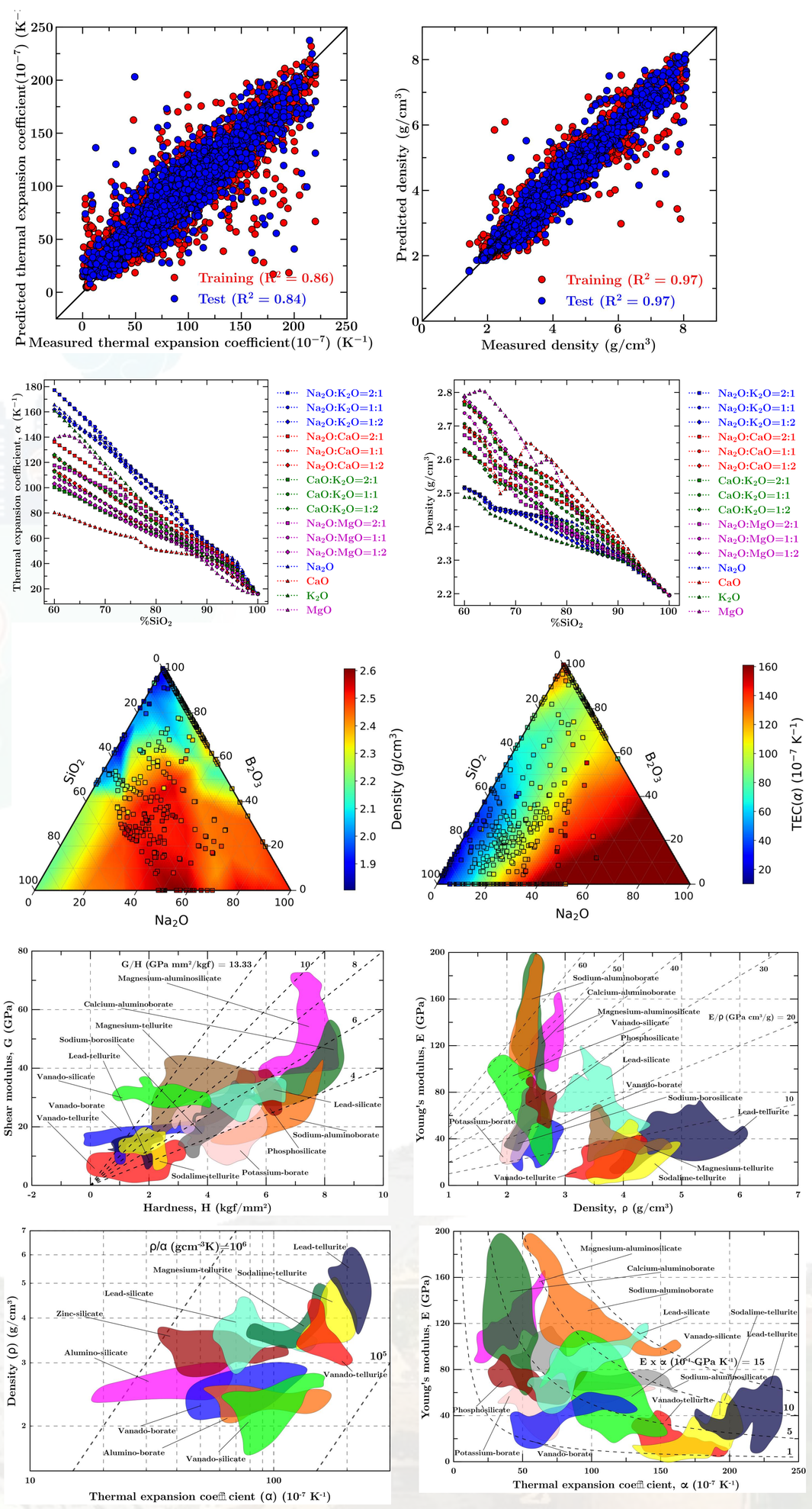
- We select density, Young's modulus, coefficient of thermal expansion, glass transition temperature, shear modulus and hardness for machine learning task.
- We use dataset from INTERGLAD v7 database which is a large database for inorganic glasses.
- We remove duplicate entries from dataset using mean value of all the duplicates within 5% of the mean value.
- We perform LARS (Least Angle Regression) to select relevant input features.
- Finally, we perform ML model training on features selected (37 oxides) by LARS.



b) Model Training

- We use neural network as over prediction model.
- First we optimize the neural network architecture where we select optimal number of hidden layers and neurons per hidden layers.
- Further, we train neural network to optimize the NN parameters.
- Note that dataset is divided into training and test set. We use training set for training the NN and test set for validation.
- Trained neural network is used for prediction of glass properties.

Result



Conclusions

- Trained neural network model can be used to predict glass properties for given composition.
- The methodology presented herein is highly transferable and can be used to develop glass compositions with tailored properties
- It can present useful insight to underlying physics for glasses.
- This process can be used to explore the properties for all the possible glass compositions.
- Glass selection charts can be used to find glass as per desired properties.

Industrial Significance

- Useful for accelerating the development of novel functional glasses.
- Significant cost reduction in the development of glasses.

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