CSCE587 Final project proposal (1-2 page)

Project Title**: Materials elasticity prediction**

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Abstract:

This project works on developing a state-of-art machine learning/deep neural network model to predict the materials' elastic property given only its composition/formula.

Backgrounds:
Currently, ordering an affordable lunch delivered to our dorm or any site on campus is not easy. There is a big niche market for affordable meal delivery service. Most restaurant apps such as xxx do not provide delivery services. Joyrun delivery service apps do not xxxx. We are aiming to develop an app for this market by providing meal delivery service..

Previously, Zhao et al. used electronic cloud as features for elasticity prediction, however, …. It is not fast enough ……

We propose to use deep neural network with convolution layers and LSTM layers for elastic property prediction

Datasets: input materials compositions/formula
Example: SrTiO3

Output: elastic property

Dataset downloaded from
https://hackingmaterials.lbl.gov/matminer/dataset_summary.html
`elastic_tensor_2015`

Evaluation:
the performance of the prediction algorithm will be evaluated using R^2, MAE, RSME