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Universal Bandgap Predictor: A Deep Learning Approach

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Bandgap and its role in advanced materials

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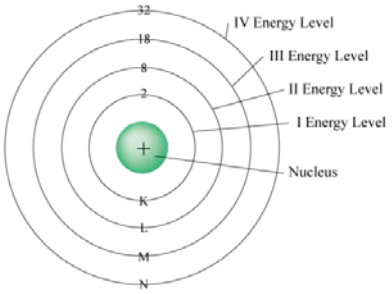
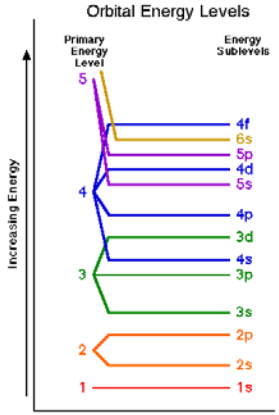
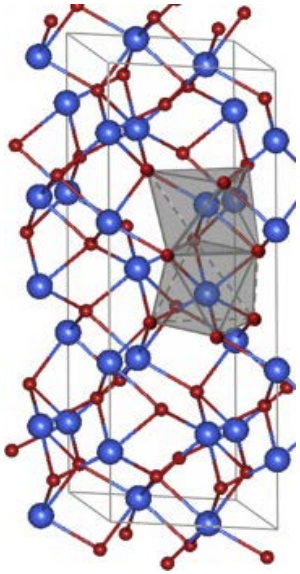
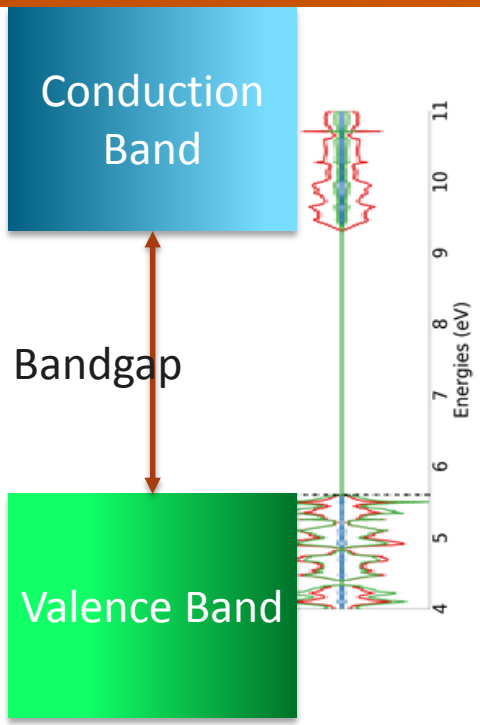


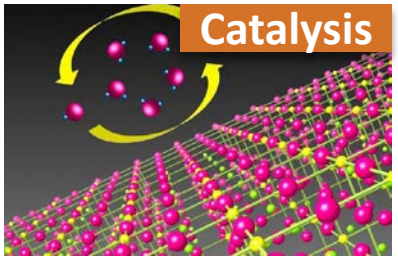


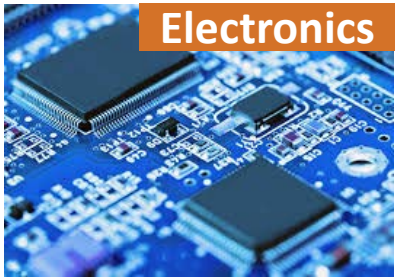


Atom Electron Levels



Crystal Electron Levels





Need for deep learning based bandgap prediction

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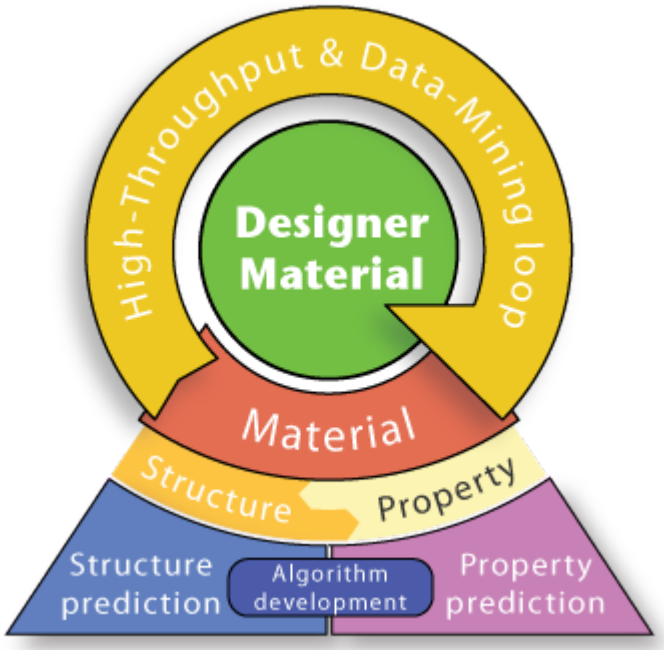
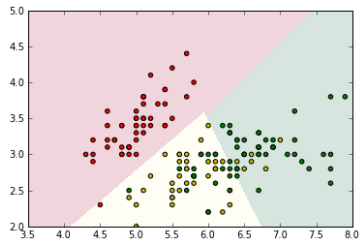
High Throughput Materials Discovery

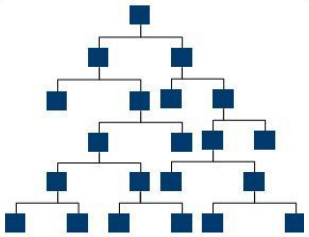


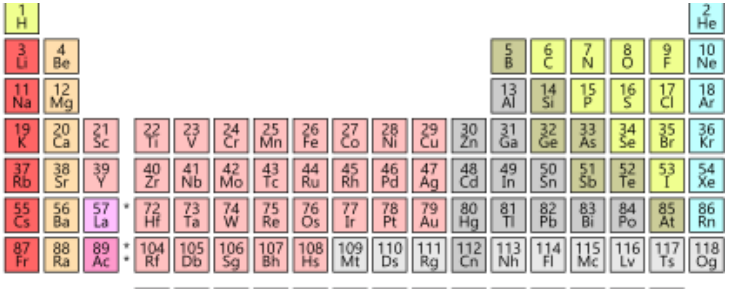
Courtesy: Gerd Ceder, LBNL and UC Berkeley

- Bandgap needs to be predicted for thousands of candidate materials simulated in silico for functional applications
- Accurate bandgap calculations are expensive

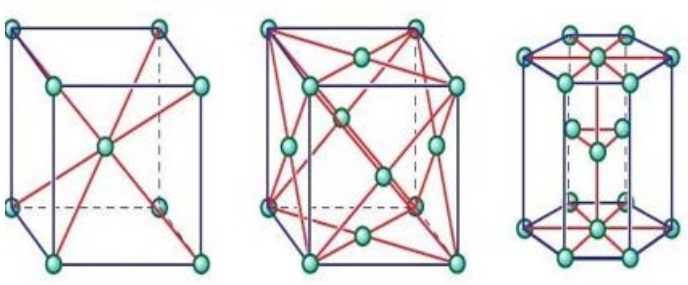
Conventional machine learning is a limiting factor







Huge variation in electronic structure and atomic/ionic radii



230 crystal symmetries

A, A_xB_y, $A_xB_yC_z$, ...

Number of elements from 1 to 6 with varying compositions

Deep Learning Approach

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Data Specifics

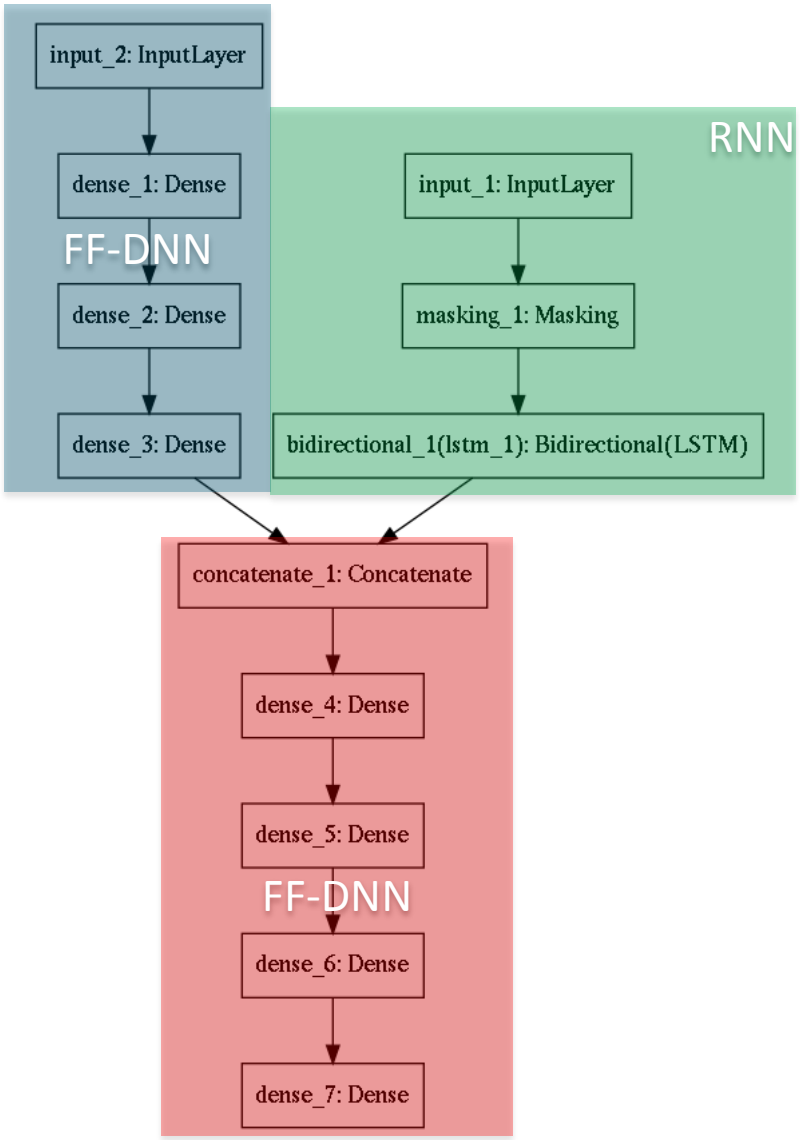
- Bandgap data for 6000 compounds (density functional theory computation)
- Crystal structure data for the compounds as well as the elemental properties

Target

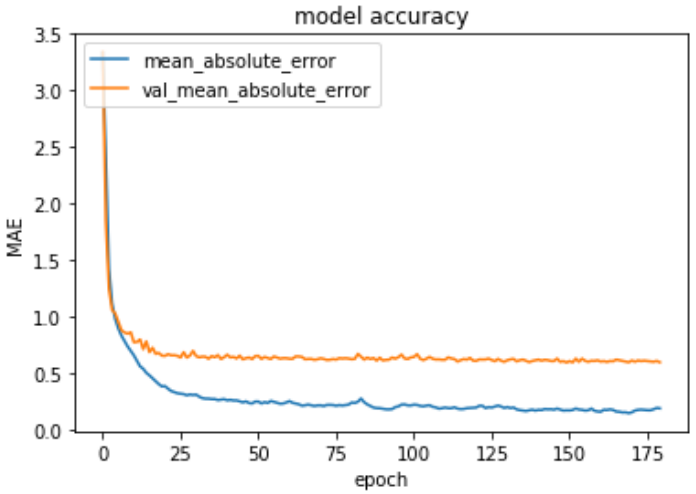
- Predict bandgap in inorganic materials with a MAE ≤ 0.3 eV

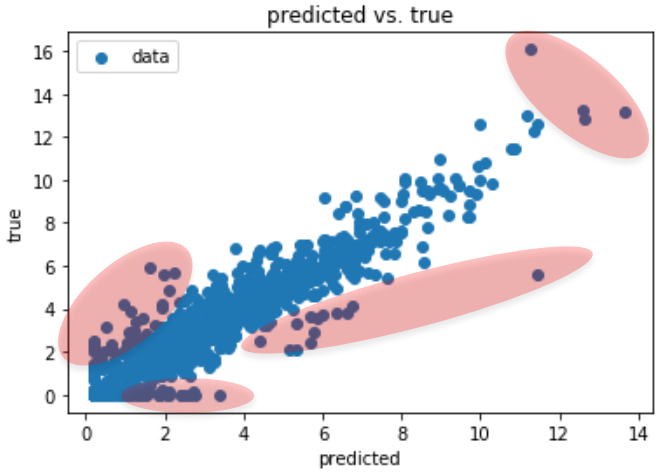
Model Details

- Hybrid model consisting of RNN for variable number of features and FF-DNN for fixed number features of the crystal
- The model uses hot-encoded elemental information and the chemical knowledge fed to the model is kept at a minimum
- From material science point of view, the model is primarily dependent on local coordination environments



Deep learning model performance





- Accuracy of MAE ~ 0.45 eV on test data (tantalizingly close!)

Improving Performance

- Inputting additional features to the model can bring the target accuracy closer to desired 0.3 eV.
- Different chemical properties can serve as distinct data representations for elements. We can try out them in a iterative fashion and find out which properties are better suited for the task at hand (equivalent to feature engineering, which we were hoping to avoid).
- Training the model on bigger datasets is another option. This will be pursued if we can't further improve the accuracy with the above two approaches.