Band Gap Prediction of 2D Materials from 3D Bulk Counterparts

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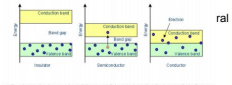
Motivation

- 2D layered materials have emerged as an important subdiscipline in nanotechnology
- The few 2D materials studied so far have shown extraordinary electrical, mechanical, thermal, and optical properties that can be utilized in fabricating next-generation transistors, sensors, and energy devices
- The band gap (Eg) of a material plays a critical role in determining its properties. 2D materials have significantly different band gaps compared to their 3D bulk counterparts
- Computational/experimental m ral networks enable fast predictive



Semiconductors, insulators and metals have a small, large and zero band gap respectively. (Source: https://www.hobbiekinder.org/en/)

Problem Definition

Use deep learning techniques to predict the band gaps of 2D materials from the properties of their 3D bulk counterparts

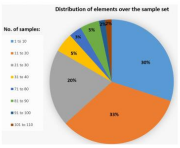
Data and Features

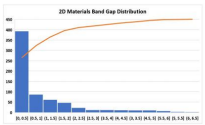
- **MLP and Linear Regression Models:** The dataset contains 666 samples (chemical compounds) of 2D materials with their PBE-calculated band gap values ranging from 0 eV to 6.5 eV

Sample Data

	Formula	3D Bulk Band Gap (eV)	3D Formation Energy (eV)	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ(°)	3D Density (g/cc)	2D Band Gap (eV)	Element1	Element2	Element3
0	AgBr	1.171	-0.372	4.476	4.476	4.476	60.000	60.000	60.000	4.92	1.724	1	1	0
1	AgCl	0.954	-0.725	3.976	3.976	3.976	60.000	60.000	60.000	5.36	1.569	1	1	0
2	AgF	0.000	-1.194	3.596	3.596	3.596	60.000	60.000	60.000	6.62	0.497	1	1	0
3	AgF2	0.000	-1.455	3.711	5.126	5.051	90.000	95.392	90.000	5.06	0.000	1	2	0
4	AgI	1.368	-0.284	4.696	4.696	4.696	60.000	60.000	60.000	5.32	1.769	1	1	0
5	AgI2	0.025	-0.052	8.782	6.355	4.286	90.004	60.790	43.648	5.15	0.000	1	2	0
6	AgO2	0.000	-0.001	7.115	7.115	7.115	64.177	135.873	135.873	5.39	0.000	1	2	0

- **Baseline Model for Transfer Learning:** This dataset contains 6105 samples of 3D bulk materials. The input features include the sample's bulk properties such as bulk band gap, density, crystal system, etc.
- **Pre-processing**: For both the models, only the most stable compound for the given composition were used





Models and Cost Functions

Linear Regression

Cost Function: $\mathcal{L} = \frac{1}{n}\sum_{i=1}^{n}(y^{(i)} - \hat{y}^{(i)})^2$

Multilayer Perceptron (MLP)

Input Layer (Size 12) → Hidden Layer (Size 8) → Output Layer (Size 1)

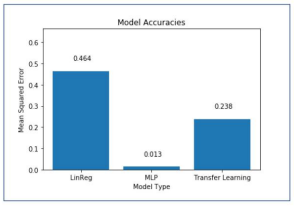
Transfer Learning

Input Layer (Size 6) → Hidden Layer (Size 4) → Hidden Layer (Size 2) → Output Layer (Size 1)

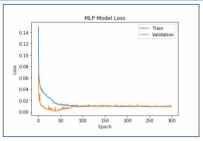
Frozen for new model | Retrained in new model

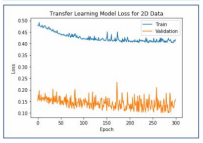
Results

Test Set Error (Mean Squared Error)

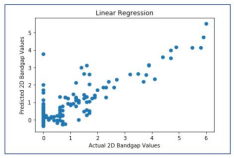


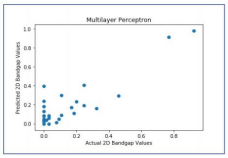
Training/Validation Error

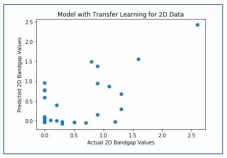




Comparison of Actual and Predicted Band Gap Values







Analysis

Model Comparison with Standard

- No comparison standard for 2D material band gaps in literature - band gap prediction has only been done for 3D materials
- Previous neural networks that predicted 3D material band gaps have had Mean Square Errors (MSE) ranging from 0.5 - 0.8 units
- All three models for the 2D dataset had lower error than the 3D prediction models - may indicate that 2D band gaps are easier to predict

Error Comparisons

	Train	Validation	Test
Linear Regression	NA	NA	0.464427
Multilayer Perceptron	0.00878316	0.00946982	0.013385
Transfer Model on 2D Bandgap Data	0.416711	0.158292	0.241689

Model Analysis

- All three models obtained their lowest MSE when optimized with the Adaptive Moment Estimation (Adam) algorithm
- Both the MLP and the model used for transfer learning were trained with mini-batches of size 32 (resulting in the spikes in the loss curves)
- Initially, the model used for transfer learning overfit the data (low training set MSE, high validation set MSE). To address this, we reduced the number of neurons in each layer
- MSE of the model used for transfer learning was higher than the MSE of the standard MLP - this may be due to the higher MSE of the MLP for the 3D dataset, since its larger size causes overfitting

Future Work

- Utilize a database that specifies the band gap type (direct/indirect) to better predict the electrical properties
- Train a Convolutional Neural Network (CNN) on a database of the band structure images to get better predictions
- Use one-hot vector encoding that uses a vector of length that equals the total number of elements present in the dataset, so the neural network can learn about each element individually

References

[1] Sten Haastrup et al 2018 *2D Mater.* 5, 042002 (2018).
[2] Jain *et al. APL Materials* 1, 011002 (2013); doi: 10.1063/1.4812323.
[3] Gowoon Cheon, Karel-Alexander N. Duerloo, Austin D. Sendek, Chase Porter, Yuan Chen, and Evan J. Reed. *Nano Lett.* 2017, 17, 1915−1923.
[4] Arunkumar Chitteth Rajan, Avanish Mishra, Swanti Satsangi, Rishabh Vaish, Hiroshi Mizuseki, Kwang-Ryeol Lee, and Abhishek K. Singh. *Chem. Mater.* 2018, 30, 4031−4038.
[5] Ya Zhuo, Aria Mansouri Tehrani, and Jakoah Brgoch. *J. Phys. Chem. Lett.* 2018, 9, 1668−1673.