Estimation of Electronic Band Gap Energy Using Machine Learning

Sagar Prakash Barad & Sajag Kumar

Using supervised learning to predict band gap energy of materials using their properties and inexpensive DFT calculations.

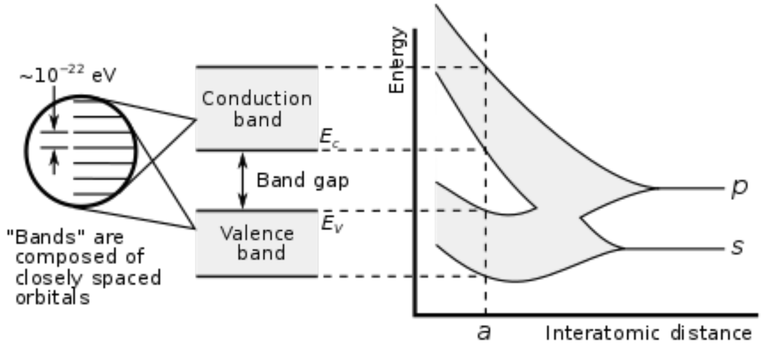

Figure credits - Band gap. (2022, November 11). In *Wikipedia*. https://en.wikipedia.org/wiki/Band_gap

Dataset(s) - The Materials Project, Automatic - FLOW for Materials Discovery (AFLOW), Computational 2D Materials Database

1. Zhang Y, Xu W, Liu G, Zhang Z, Zhu J, Li M (2021) Bandgap prediction of two-dimensional materials using machine learning. PLoS ONE 16(8): e0255637. https://doi.org/10.1371/journal. pone.0255637.
2. Dong Y, Wu C, Zhang C, Liu Y, Cheng J, Lin J (2019) Bandgap prediction in configurationally hybridised graphene and boron nitride, npj Computational Materials (2019)5:26 ; https://doi.org/10.1038/s41524-019-0165-4.

Work division upto mid-term presentation.

#TODO	To be done by...
Literature Review	Both
Slides and Reports	Sajag
Data Analysis & Visualisation	Sagar
Implementation of ML Algorithms	Both

Midway Targets

1. Come up with a consistent set of features/classification scheme for different types of materials.
2. Implement classic machine learning algorithms to achieve the current state-of-the-art results.
3. Perform ensemble learning to improve upon the hitherto achieved results.

Expected Results

1. Performance of ML algorithms: as good as in case of specific types of materials.
2. Ensemble learning: better results than the individual algorithms.