Band-gap Prediction

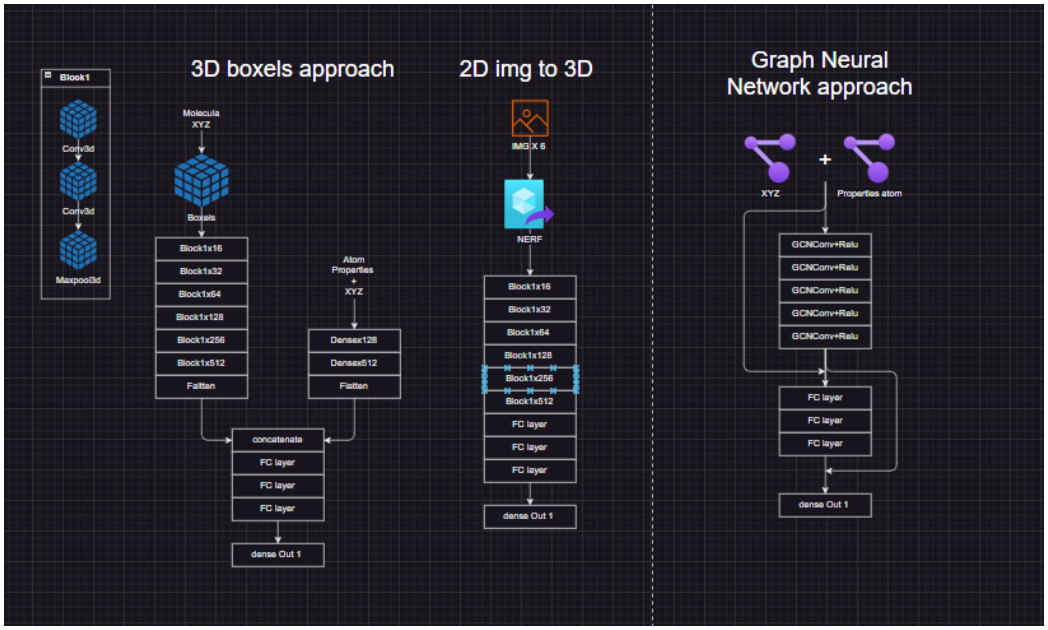
Band-gap, also known as energy band gap, refers to the energy difference between the valence band (the highest energy level of electrons in a material that are still bound to an atom) and the conduction band (the lowest energy level of electrons that are free to move around in a material and conduct electricity).

The size of the band-gap determines whether a material is an insulator, semiconductor or conductor. Insulators have a large band-gap and do not conduct electricity well, whereas conductors have a small band-gap and conduct electricity easily. Semiconductors have a band-gap in between insulators and conductors, and their electrical conductivity can be controlled by varying their band-gap through the addition of impurities or by changing their temperature.

The band-gap is an important property of materials and plays a crucial role in the development of electronic devices such as transistors, solar cells, and light-emitting diodes (LEDs).

The objective of the paper is to provide an overview of the experimental and theoretical methods used to predict the band-gap of materials, and to compare their advantages and disadvantages. This paper aims to explain the importance of band-gap prediction in materials science and electronic device applications, and to highlight the challenges involved in accurately predicting band-gaps.

Possible architectures



The first one is base in boxes providing a 3d space with every boxel fill with N properties similar to nerf RGB boxel, also adding XYZ coordinates and property of atoms in an extra input

The second architecture use a full nerf model receiving input of 6 images one per every side of the particle in a cube an try to infer the properties and connections in the molecule to predict the band-gap

The last possible architecture use Graph Neural Networks to get the spatial data XYZ and the atom properties to try to find de Edges of the molecule and then get the band gap prediction