Review 1: [IDAO 2022 Qualifying Round Task Presentation (Konstantin Novoselov, Abdalaziz Al-Maeeni)](https://www.youtube.com/watch?v=pzv_XIIatB8&list=PLEqoHzpnmTfCyU01RD4Ad05AkozaNqh0p)

Abstract:

Graphical neural networks (GNNs) have attracted a great deal of interest as a fast-growing class of machine learning models that are remarkably well-suited to materials applications. To date, a number of successful GNNs have been proposed and demonstrated for systems ranging from crystal stability and electronic property prediction to surface chemistry and heterogeneous catalysis. In particular, GNNs could be used for predicting properties of molecules based on graphene.

Introduction:

GNN has emerged as a powerful new tool in materials science, driven in part by the advent of large materials data sets from high-throughput electronic structure calculations and/or combinatorial experiments. Among its many applications, the evelopment of fast, surrogate GNN models for property prediction has arguably received the most interest for its potential in accelerating materials design as well as accessing larger length/time scales at near-quantum accuracy.

Body:

Band gap is one of the important physical attributes which describe certain characteristics of the material, that helps deriving material qualities including electric conductivity or catalytic power or photo-optical properties. Band gap is the energy difference between the valence band and conduction band and is closely related to the energy difference between highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), materials with overlapping (between valence band and conduction band) or very small band gap are conductors and materials with small bandgap are semiconductors while materials with large bandgap are insulators.

Provided with atomic structures and target properties from any dataset of choice, GNN handles the processing of structures to graphs, and provides hyperparameter optimization for the models. Within this framework, improvements and additions to the input representations and model architectures can be easily made, which can greatly reduce the development time needed for new ML models. GNNs can also be critically evaluated, and actionable information can be quickly obtained when applied to specific problems in chemistry and the materials sciences.

Conclusion:

To conclude, materials graph network models that are universally high performing across a broad variety of target properties for both molecules and crystals. Graphs are a natural choice of representation for atoms and the bonds between them, and he sequential update scheme of graph networks provide a natural approach for information

flow among atoms, bonds and global state.

Discussion:

I think GNN model aimed to predict material properties by its molecular structure is a of great significance for the future of chemistry and materials science, and provide a robust foundation for the development of general property models for accelerating new materials discovery.