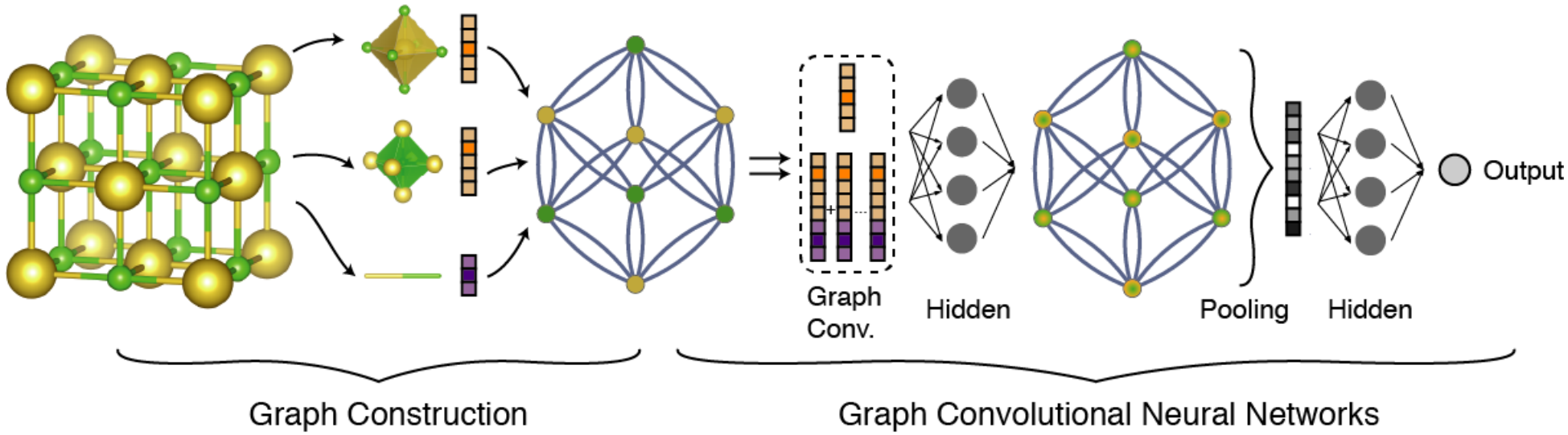
CGCNN: a graph representation of materials for property prediction and materials design



- A framework to learn structure-property relations for arbitrary periodic materials.
- DFT accuracy prediction of 8 material properties with 10^4 acceleration.
- Understand material similarities at different scales from the neural networks.
- Two use cases of screening inorganic and polymer materials for electrolytes in batteries.

T. Xie, J. Grossman. *Phys. Rev. Lett.* 120, 145301, 2018
Z. Ahmad, **T. Xie**, et al. *ACS Cent. Sci.* 4, 996, 2018
T. Xie, J. Grossman, *J. Chem. Phys.*, in press.

Code open source at https://github.com/txie-93/cgcnn