Crystal graph convolutional neural networks for condensed matter physics and material science

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In recent years Machine Learning techniques have come of age, finding a very wide range of applications across industry and science. In particular, Deep Learning, the branch of Machine Learning that is concerned with the design, training and exploitation of Artificial Neural Networks (ANNs), has demonstrated the ability to address problems that were intractable with previously available methods, such as near-human level image classification, speech recognition, handwriting transcription, autonomous driving, among many others.

The aim of this project is to explore the application of graph convolutional neural networks for accelerating the design and theoretical analysis of crystalline materials. Using training sets obtained from open-source databases or from in-house DFT calculations, we will study how to build convolutional neural networks on top of crystal graphs generated from crystal structures in order to predict selected properties (energy, polarizability, hardness, etc). We will also explore the possibility of using *generative* graph neural networks in order to create new crystal structures with desirable properties. This field of research is at the cutting edge of the application of Artificial Intelligence techniques to Materials Science and Condensed Matter Physics.

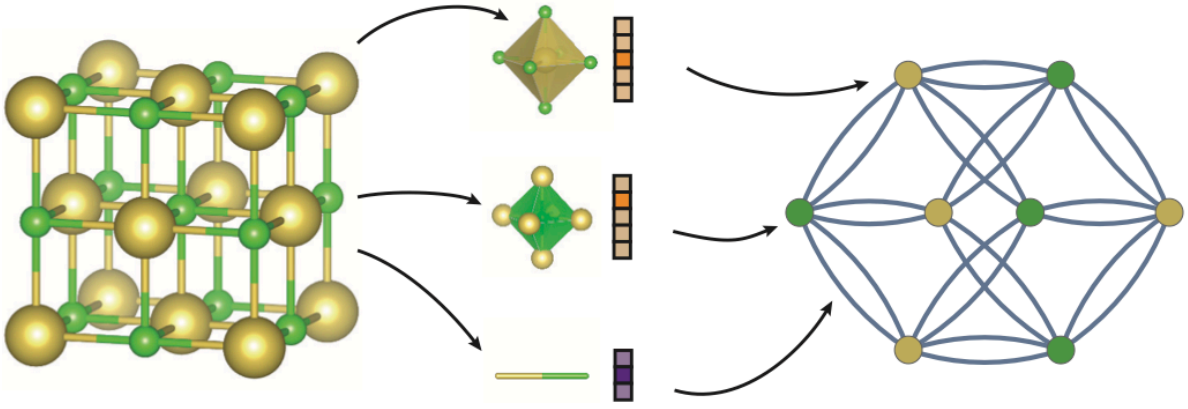

Figure 1. Schematics of graph convolutional neural network generated from the unit cell of a crystal.

References:

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