Prediction of Quantum Materials for Environmental Gas Monitoring

Paul C.H. Li *
Department of Chemistry, Simon Fraser University (SFU), Burnaby, British Columbia, Canada

Sepehr Roonasi
Department of Chemistry, Simon Fraser University (SFU), Burnaby, British Columbia, Canada

Ka Ho Wong
Department of Chemistry, Simon Fraser University (SFU), Burnaby, British Columbia, Canada

Shabnam Rehmat
Department of Chemistry, Simon Fraser University (SFU), Burnaby, British Columbia, Canada

Abstract

The recently discovered topological insulator (TI) exhibits quantum properties of uni-directional edge electrical conduction that favor measurements with high signal/noise ratio. These materials are favorable for highly sensitive and selective environmental monitoring for gases such as NO_2. The materials properties of known TIs, such as Bi_2Se_3, will be used in machine learning (ML) in artificial intelligence (AI) to train the convoluted neural network (CNN) used in deep learning. To optimize sensor performance, new TI materials will be predicted using CNN. This has accelerated material designs by properties prediction with near *ab initio* accuracy at much faster speed. A trained orbital graph convolutional neural network (OGCNN) has been adapted to accurately predict different crystals with various structure types and compositions. The material properties include formation energy, band gap, Fermi energy, spin-orbital coupling spillage, etc.

The material structure is represented by a crystal graph. The atom features include group and period numbers, valence electrons, ionization energy, electron affinity, atomic volume; the bond feature includes atom distance. In addition, the orbital-orbital interactions are also included by the two-dimensional descriptor called the orbital field matrix (OFM). The inclusion of these interactions to encode the local chemical environments of atoms along with embedding of an encoder-decoder network enabled the OGCNN to achieve higher accuracy for prediction of new topological quantum sensing materials.