Application of machine learning for materials with targeted properties

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Abstract

The integration of machine learning(ML) into materials science has revolutionized our ability to design materials with tailored properties, unlocking new frontiers in material optimization and innovation. This proposed talk explores applications of machine learning in achieving targeted material properties. The first example introduces a machine learning assisted workflow in predicting magnetic double perovskites[1]. This has led to filtering out of 25 stable structures for their detailed characterization. Two of the predicted double perovskites have been recently synthesized and would be communicated shortly. We have further derived the electronic and magnetic nature of the predicted compounds using first principles calculations. In the next example, viable candidates for rare earth-lean permanent magnets, which find applicability in almost every important technology, have been anticipated using a combination of machine learning and first-principles calculations[2]. The algorithm has been trained to make predictions on magnetic transition temperature (T_c), largeness of saturation magnetization ($\mu_0 M_s$), and the nature of the magnetocrystalline anisotropy (K_u) – the three cornerstones of a good permanent magnet. The third work involves semiconductor heterostructures, particularly, its type derived from the bandstructures of the constituent semiconductors[3]. In another work, we have delved into the domain of nanoscale binary metal alloys to investigate the driving factors determining their core-shell preference[4]. In the final example we have utilized ML in developing a microscopic understanding of formation of atomic wires of appreciable length by using experimentally obtained data in training[5]. Using a supervised learning scheme, we have found optimal conditions for chain formation. We have further applied an unsupervised learning scheme for the classification of individual breaking traces, thus identifying junction structures associated with longer chains. Our findings are corroborated by ab-initio molecular dynamics simulations.

References

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