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Abstract

My research topic consists of "machine learning(ML)", which originates from information science, and "density functional theory (DFT)", which is the standard method in materials science. As this kind of combination has recently been appeared, there are limited number of people familiar with this topic. To improve my understanding about this topic, I applied for the ISSP research travel program to visit Prof. Kieron Burke in UCI, who is a pioneer of this "ML + DFT" as well as an expert of basic studies of DFT.

Research

Conventional density functionals have been developed through heuristic way; they compare performances of functionals constructed using various combination of physical conditions. Meanwhile, using ML, we demonstrated that a functional can be constructed with comparable performance to conventional ones. However, to improve our method and construct better functionals, many details are yet to be uncovered. In my stay in UCI, Prof. Burke suggested approaches to investigate the basic properties of our ML functionals. As the results of our research, many properties of this method were revealed, and we found some important strategies to construct accurate ML functionals.

Life in Irvine

While staying in Burke group, I attended the DFT class with the student there. As Prof. Burke is well known for the expert of DFT, the quality of his lecture was actually high. I could get many insights about basics of DFT, which would not be written in the usual textbooks.
I felt that people in Irvine are highly educated and behaves well. This might be related to the fact that most people there are working in the university or leading companies.

Acknowledgement

Laguna beach and clear sky of California.