11:15 a.m. BU 120 – Sean Stein Pavilion Auditorium

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"Machine Learning for Materials Science"

Abstract: In recent years, machine learning has emerged as a distinct tool for the design and characterization of materials. Especially, the progress of computing power and algorithms, together with the availability of large amount of data obtained from high-throughput quantum mechanical calculations, brings new opportunities for enabling accelerated materials discovery. In this presentation, I will show an upcoming NSF supercomputing facility at Pittsburgh Computing Center which is designed to assist AI and machine learning research activities for academic communities. For machine learning applications, I will discuss the importance of high-performance computing environment and show how the data-to-knowledge transfer enables the characterization of multicomponent random alloys.